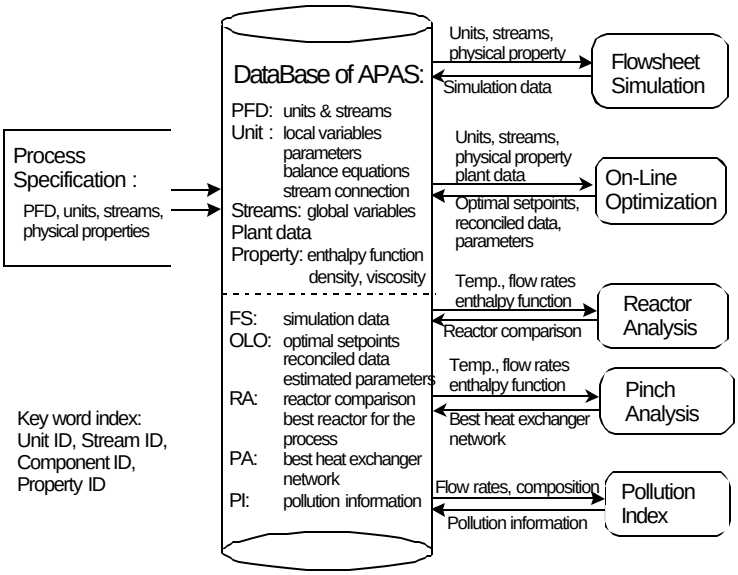

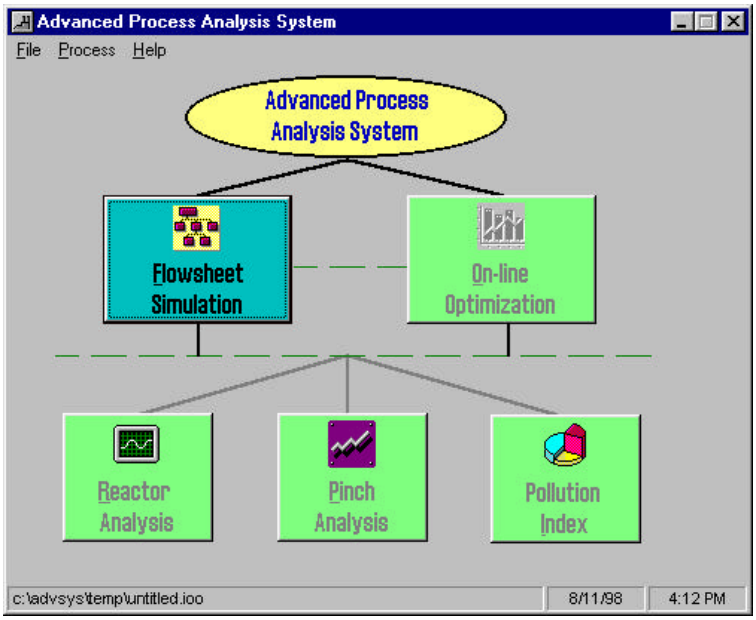

Mineral Processing Research Institute

Louisiana State University

Advanced Process Analysis System

User's Manual
and
Tutorial
for the Aniline Process

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March 1,2001

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I. INTRODUCTION AND METHODOLOGY

The Advanced Process Analysis System is a powerful tool for use by process and plant engineers to perform comprehensive and in-depth evaluations of economic, environmental, safety and hazard analysis projects. This system is based on chemical engineering fundamentals such as stoichiometry, thermodynamics, fluid dynamics, heat transfer, mass transfer, reactor design and optimization. It helps identify pollutants in chemical processes and petroleum refineries and develop innovative, economically viable designs to eliminate their generation. It aims at waste minimization and pollution prevention in chemical plants, in addition to increased profit and improved efficiency of operations.

The framework of the Advanced Process Analysis System is shown in Figure 1. The main components of this system are a flowsheeting program for process material and energy balances, an on-line optimization program, a chemical reactor analysis program, a heat exchanger network design program, and a pollution assessment module. A Windows interface is used to integrate these programs into one user-friendly application.

The Advanced Process Analysis System methodology to identify and eliminate the causes of energy inefficiency and pollutant generation is based on the onion skin diagram shown in Figure 2. Having an accurate description of the process from on-line optimization, an evaluation of the best types of chemical reactors is done first to modify and improve the process. Then the separation units are evaluated. This is followed by the pinch analysis to determine the best configuration for the heat exchanger network and determine the utilities needed for the process. Not shown in the diagram is the pollution index evaluation, which is used to identify and minimize emissions. The following gives a detailed description of the Advanced Process Analysis System and its components, and how they are used together to control and modify the process to maximize the profit and minimize the wastes and emissions. An aniline process simulation is used as a tutorial process to demonstrate the use and capabilities of the Advanced Process Analysis System. This will follow the description of the programs and the components. The separate manual is available for the contact process for sulfuric acid manufacture. It is for an actual plant, and the workstation version of GAMS is required for on-line optimization.

A. Flowsheeting

The first step towards implementing the Advanced Process Analysis System is the development of the process model using Flowsim. As described earlier, the process model is a set of constraint equations, which are the material and energy balances, rate equations and equilibrium relations that describe the material and energy transport and the chemical reactions of the process. These form a mathematical model of relationships between the various plant units and process streams. Formulation of the process model can be divided into two important steps.

A-1. Formulation of Constraints for Process Units

The formulation of constraints can be classified into empirical and mechanistic methods.

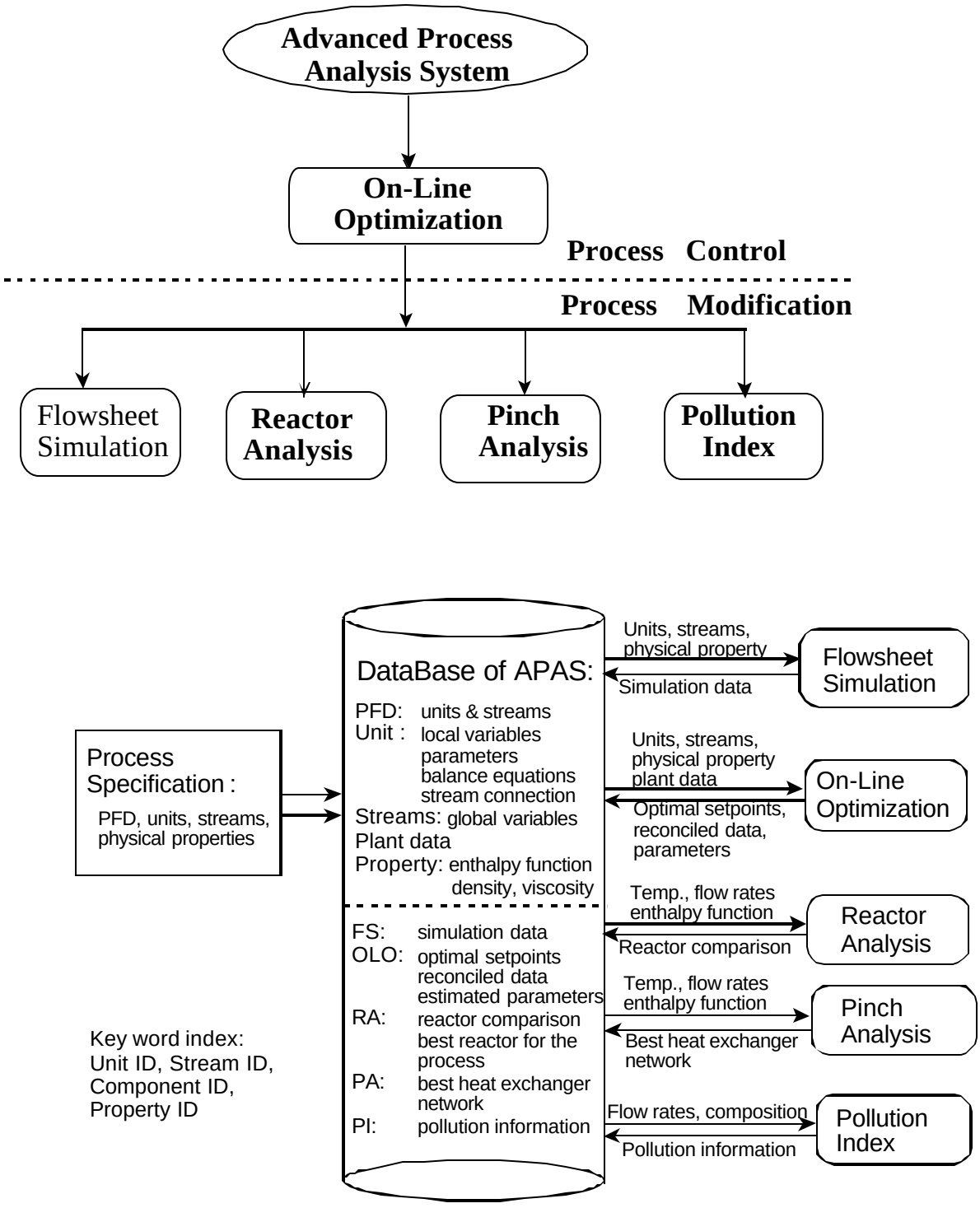


Figure 1. The Framework of the Advanced Process Analysis System

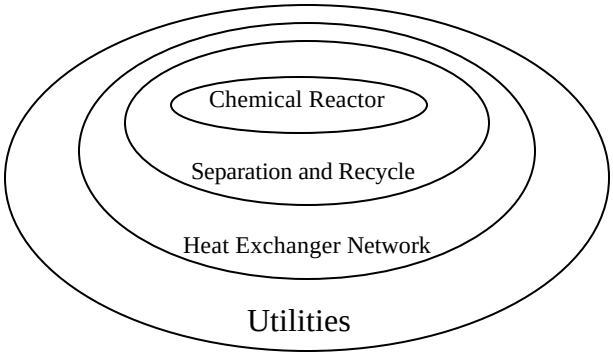


Figure 2. The 'Onion Skin' Diagram for Organization of a Chemical Process and Hierarchy of Analysis.

The process models used in Advanced Process Analysis System belong to the type of mechanistic models because they are based on conservation laws as well as the physical and chemical attributes of its constituents.

A typical chemical plant includes hundreds of process units such as heat exchangers, reactors, distillation columns, absorption towers and others. The constraints for these units are either based on conservation laws (mass and energy balances) or they are based on some other laws of nature which include models for chemical phase equilibrium, kinetic models etc. Mathematically, the constraints fall into two types: equality constraints and inequality constraints. Equality constraints deal with the exact relationships such as material and energy balances in the model. The inequality constraints recognize the various bounds involved. Examples of inequality constraints are upper limits on the temperature of certain streams or upper limits on the capacity of certain units.

A-2. Classification of Variables and Determination of Parameters

After the constraints are formulated, the variables in the process are divided into two groups, measured variables and unmeasured variables. The measured variables are the variables which are directly measured from the distributed control systems (DCS) and the plant control laboratory. The remaining variables are the unmeasured variables. For redundancy, there must be more measured variables than the degree of freedom.

The parameters in the model can also be divided into two types. The first type of parameters is the constant parameters, which do not change with time. Examples of these are reaction activation energy, heat exchanger areas etc. The other type of parameters is the time-varying parameters such as catalyst deactivation and heat exchanger fouling factors. These are treated as parameters because they change very slowly with time. They are related to the equipment conditions and not the operating conditions.

A-3. Flowsim Interface

Flowsim is used to develop the process model, and it has a graphical user interface with interactive capabilities. Process units are represented as rectangular shapes whereas the process streams are represented as lines with arrows between these units. Each process unit and stream

included in the flowsheet must have a name and a description. Process information is divided into the following six categories: equality constraints, inequality constraints, unmeasured variables, measured variables, parameters and constants.

The information in the first five categories is further classified by associating it with either a unit or a stream in the flowsheet. For example, for a unit that is a heat exchanger, the relevant information includes the mass balance and heat transfer equations, limitations on the flowrates and temperatures if any, the heat transfer coefficient parameter and all the intermediate variables defined for that exchanger.

For a stream, the information includes its temperature, pressure, total flowrate, molar flowrates of individual components etc. Also, information not linked to any one unit or stream is called the 'Global Data'. For example, the overall daily profit of the process is a global unmeasured variable.

The sixth category of constants can be grouped into different sets based on their physical significance. For example, constants related to heat exchangers can be placed in one group and those related to reactors into another group.

Flowsim also has a seventh category of information called as the 'enthalpy coefficients'. This stores the list of all the chemical components in the process and their enthalpy coefficients for multiple temperature ranges. All of this process information is entered with the help of the interactive, user-customized graphic screens of Flowsim. The formulation of process models and the classification of process information for the aniline process is given in Section II. The next step of Advanced Process Analysis System is on-line optimization.

B. The Online Optimization Program

Once the process model has been developed using Flowsim, the next step is to conduct on-line optimization. On-line optimization is the use of an automated system which adjusts the operation of a plant based on product scheduling and production control to maximize profit and minimize emissions by providing setpoints to the distributed control system. As shown in Figure 3, it includes three important steps: combined gross error detection and data reconciliation, simultaneous data reconciliation and parameter estimation and plant economic optimization. In combined gross error detection and data reconciliation, a set of accurate plant measurements is generated from plant's Distributed Control System (DCS). This set of data is used for estimating the parameters in plant models. Parameter estimation is necessary to have the plant model match the current performance of the plant. Then the economic optimization is conducted to optimize the economic model using this current plant model as constraints and this generates the optimal setpoints for the Distributed Control System.

Each of the above three optimization problems in on-line optimization has a similar mathematical statement as following:

Optimize: *Objective function*
Subject to: *Constraints from plant model.*

where the objective function is a joint distribution function for data validation or parameter estimation and a profit function (economic model) for plant economic optimization. The constraint equations describe the relationship among variables and parameters in the process, and they are material and energy balances, chemical reaction rates, thermodynamic equilibrium relations, and others.

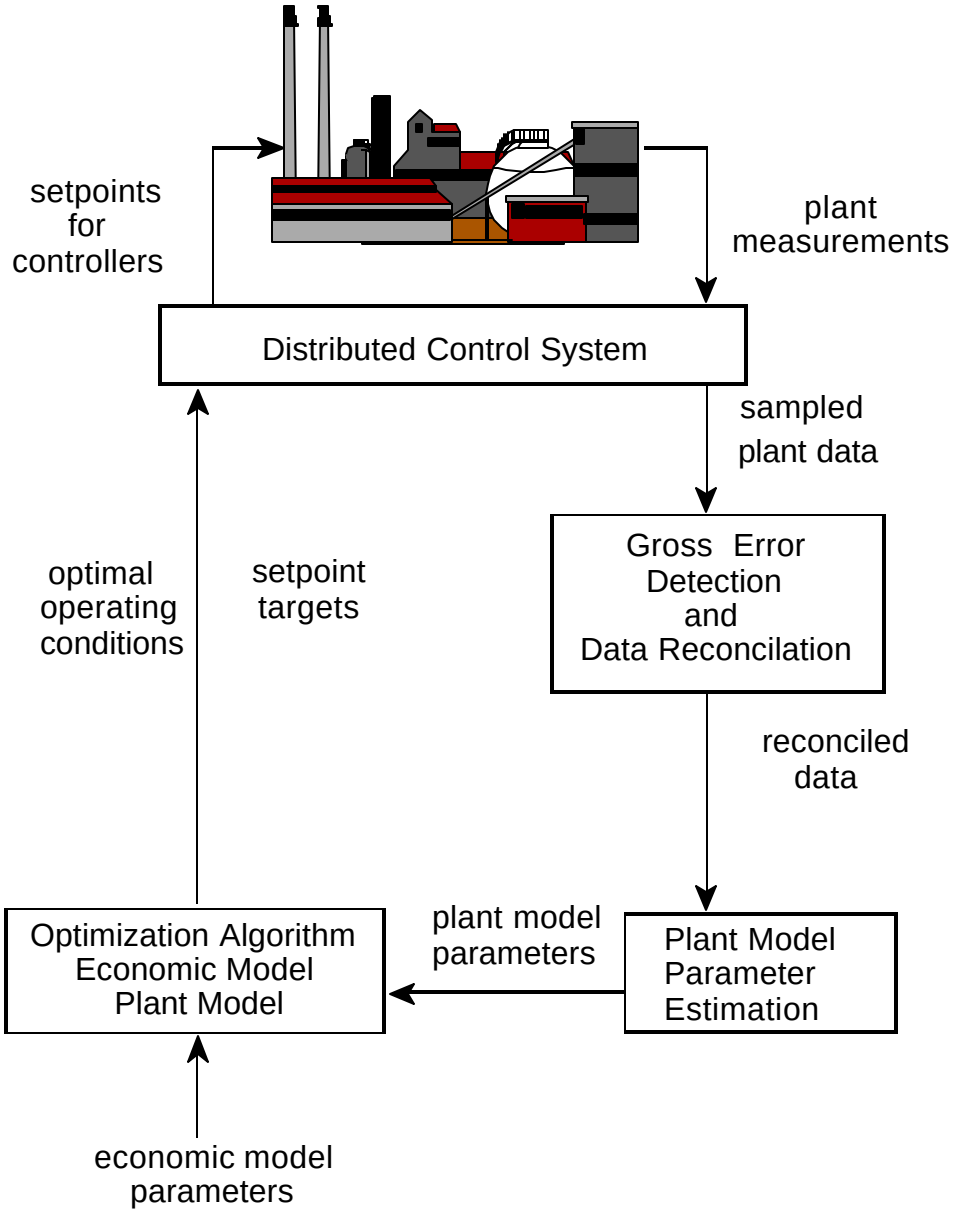


Figure 3. Simplified Structure of Online Optimization

To perform data reconciliation, there has to be more measurements than necessary to be able to rectify errors in instruments. For redundancy, the number of measurements to determine the unmeasured variables is given by the degree of freedom, which is calculated using the following equation.

Degree of freedom = Total number of variables – Total number of equality constraints + Number of chemical reactions

Also, the unmeasured variables have to be determined by the measured variables, called observability. If an unmeasured variable can not be determined by a measured variable, it is unobservable. This is called the 'observability and redundancy criterion', which needs to be satisfied.

B-1. Combined Gross Error Detection and Data Reconciliation

The process data from distributed control system is subject to two types of errors, random error and gross error, and the gross error must be detected and rectified before the data is used to estimate plant parameters. Combined gross error detection and data reconciliation algorithms can be used to detect and rectify the gross errors in measurements for on-line optimization. These algorithms are measurement test method using a normal distribution, Tjoa-Biegler's method using a contaminated Gaussian distribution, and robust statistical method using robust functions. The theoretical performance of these algorithms has been evaluated by Chen, 1998.

Based on Chen's study, the Tjao-Biegler's method is the best for chemical processes and is used to perform combined gross error detection and data reconciliation. When gross errors are in the range of $-\sigma$ to σ, it detects and rectifies gross errors in plant data sampled from distributed control system. This step generates a set of measurements containing only random errors. Then, this set of measurements is used for simultaneous parameter estimation and data reconciliation using the least squares method. This step provides the reconciled data and the updated parameter values in the plant model for economic optimization. Finally, optimal set points are generated for the distributed control system from the economic optimization using the updated plant and economic models. This optimal procedure can be used for any process to conduct on-line optimization.

B-2. Simultaneous Data Reconciliation and Parameter Estimation

The general methodology for this is similar to the methodology of combined gross error detection and data reconciliation. The difference is that the parameters in plant model are considered as variables along with process variables in simultaneous data reconciliation and parameter estimation rather than being constants in data reconciliation. Both process variables and parameters are simultaneously estimated. Based on Chen's study, the least squares algorithm is used to carry out the combined gross error detection and data reconciliation. The data set produced by the parameter estimation is free of any gross errors, and the updated values of parameters represent the current state of the process. These parameter values are now used in the economic optimization step.

B-3. Plant Economic Optimization

The objective of plant economic optimization is to generate a set of optimal operating setpoints for the distributed control system. This set of optimal setpoints will maximize the plant profit, satisfy the current constraints in plant model, meet the requirements for the demand of the product and availability of raw materials, and meet the restriction on pollutant emission. This optimization can be achieved by maximizing the economic model (objective function) subject to the process constraints. The objective function can be different depending on the goals of the optimization. The objectives can be to maximize plant profit, optimize plant configuration for energy conservation, minimize undesired by-products, minimize the waste/pollutant emission, or a combination of these objectives. The result of the economic optimization is a set of optimal values for all the measured and unmeasured variables in the process. These are then sent to the distributed control system (DCS) to provide setpoints for the controllers.

The on-line optimization program of the Advanced Process Analysis System retrieves the process model and the flowsheet diagram from Flowsim. Additional information needed to run online optimization includes plant data and standard deviation for measured variables; initial guess values, bounds and scaling factors for both measured and unmeasured variables; and the economic objective function. The program then constructs the three optimization problems and uses GAMS (General Algebraic Modeling System) to solve them. Results of all three problems can be viewed using the graphical interface of Flowsim.

The aniline process will be used to demonstrate the use and capabilities of the on-line optimization program. This is described in Section VI.

C. The Chemical Reactor Analysis Program

Having optimized the process operating conditions for the most current state of the plant, the next step in the Advanced Process Analysis System is to evaluate modifications to improve the process and reduce emission and energy consumption. First, the chemical reactors in the process are examined. The reactors are the key units of chemical plants. The performance of reactors significantly affects the economic and environmental aspects of the plant operation. The formulation of constraints in these types of units is very important and complicated owing to the various types of reactors and the complex reaction kinetics. Unlike a heat exchanger whose constraints are similar regardless of types of equipment, there is a great variation in deriving the constraints for reactors.

The chemical reactor analysis program of the Advanced Process Analysis System is a comprehensive, interactive computer simulation that can be used for modeling various types of reactors such as Plug Flow, CSTR and Batch reactors. This is shown in Figure 4. Reaction phases included are homogeneous gas, homogeneous liquid, catalytic liquid, gas-liquid etc. The options for energy model include isothermal, adiabatic and non-adiabatic.

The kinetic data needed for the reactor system includes the number of reactions taking place in the reactor and the number of chemical species involved. For each reaction, the stoichiometry and reaction rate expressions also need to be supplied. The physical properties for

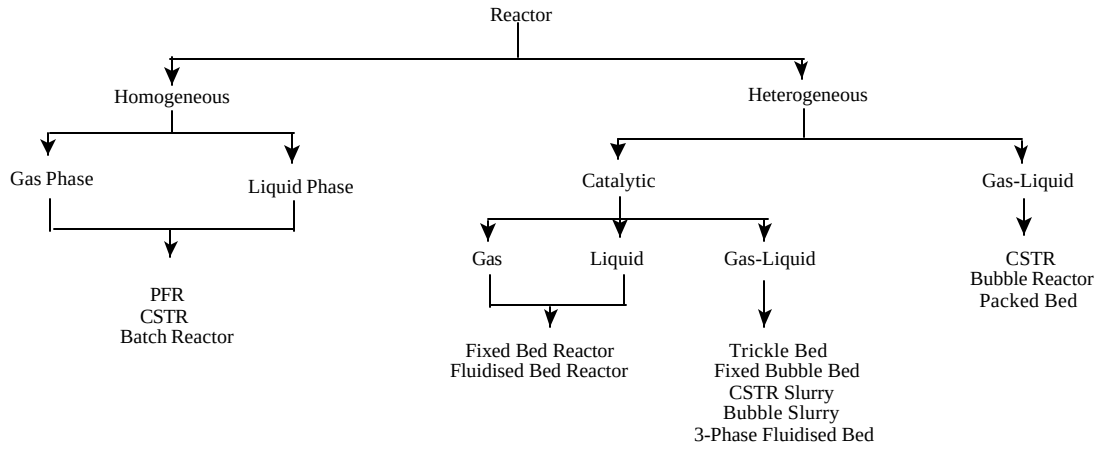


Figure 4. The Reactor Analysis Program Outline

the chemical species can be retrieved from Flowsim.

The kinetic data needed for the reactor system includes the number of reactions taking place in the reactor and the number of chemical species involved. For each reaction, the stoichiometry and reaction rate expressions also need to be supplied. The physical properties for the chemical species can be retrieved from Flowsim.

The feed stream for the reactor is obtained from Flowsim and its temperature, pressure, flowrate and composition are retrieved using the results from on-line optimization. Finally, the dimensions of the reactor and heat transfer coefficients are supplied. All of this data is used with various types of reactors to predict their performance and select the best one. The reactant concentration, conversion, temperature and pressure are calculated as function of reactor length or space-time. The results can be viewed in both tabular and graphical form.

As the operating process conditions change, the performance of the reactors also can vary to a significant extent. The reactor design program provides a tool to develop an understanding of these relationships. It provides a wide range of different types of reactors, which can be examined and compared to decide the best reactor configuration for economic benefits and waste reduction.

The aniline process will be used to demonstrate the use and capabilities of the chemical reactor analysis program. This is described in Section IX.

D. The Heat Exchanger Network Program

The optimization of the chemical reactors is followed by the heat exchanger network optimization as shown in the onion skin diagram in Figure 2. Most chemical processes require the heating and cooling of certain process streams before they enter another process unit or are released into the environment. This heating or cooling requirement can be satisfied by matching of these streams with one another and by supplying external source of heating or cooling. These

external sources are called as utilities, and they add to the operating cost of the plant. The Heat Exchanger Network program aims at minimizing the use of these external utilities by increasing energy recovery within the process. It also synthesizes a heat exchanger network that is feasible and has a low investment cost.

There are several ways of carrying out the above optimization problem. Two of the most important ones are the pinch analysis and the mathematical programming methods. Pinch analysis is based on thermodynamic principles whereas the mathematical methods are based on mass and energy balance constraints. The Heat Exchanger Network Program (abbreviated as THEN) is based on the method of pinch analysis (Knopf, 1989).

The first step in implementation of THEN is the identification of all the process streams, which are important for energy integration. These important streams usually include streams entering or leaving heat exchangers, heaters and coolers. The flowsheeting diagram of Flowsim can be an important aid in selection of these streams.

The next step in this optimization task involves retrieval of the necessary information related to these streams. Data necessary to perform heat exchanger network optimization includes the temperature, the flowrate, the film heat transfer coefficient and the enthalpy data. The enthalpy data can be in the form of constant heat capacities for streams with small temperature variations. For streams with large variations, it can be entered as temperature-dependent enthalpy coefficients. The film heat transfer coefficients are needed only to calculate the areas of heat exchangers in the new network proposed by THEN.

The temperature and flowrates of the various process streams are automatically retrieved from the results of online optimization. The setpoints obtained after the plant economic optimization are used as the source data. The physical properties such as the heat capacities, enthalpy coefficients and film heat transfer coefficients are retrieved from the Flowsim.

The third step in the heat exchanger network optimization is classification of streams into hot streams and cold streams. A hot stream is a stream that needs to be cooled to a lower temperature whereas a cold stream is a stream that needs to be heated to a higher temperature. Usually, streams entering a cooler or the hot side of a heat exchanger are the hot streams whereas streams entering through a heater or the cold side of a heat exchanger are the cold streams. The final step in this problem requires the specification of the minimum approach temperature. This value is usually based on experience.

Having completed all of the above four steps, the heat exchanger network optimization is now performed using THEN. Thermodynamic principles are applied to determine the minimum amount of external supply of hot and cold utilities. The Composite Curves and the Grand Composite Curve are constructed for the process. These curves show the heat flows at various temperature levels. Illustrations of the composite curves are given in Figure 5. A new network of heat exchangers, heaters and coolers is proposed, which features the minimum amount of external utilities. This network drawn in a graphical format is called the Network Grid Diagram. An example of a network grid diagram is given in Figure 6. Detailed information about the network can be viewed using the interactive features of the user interface.

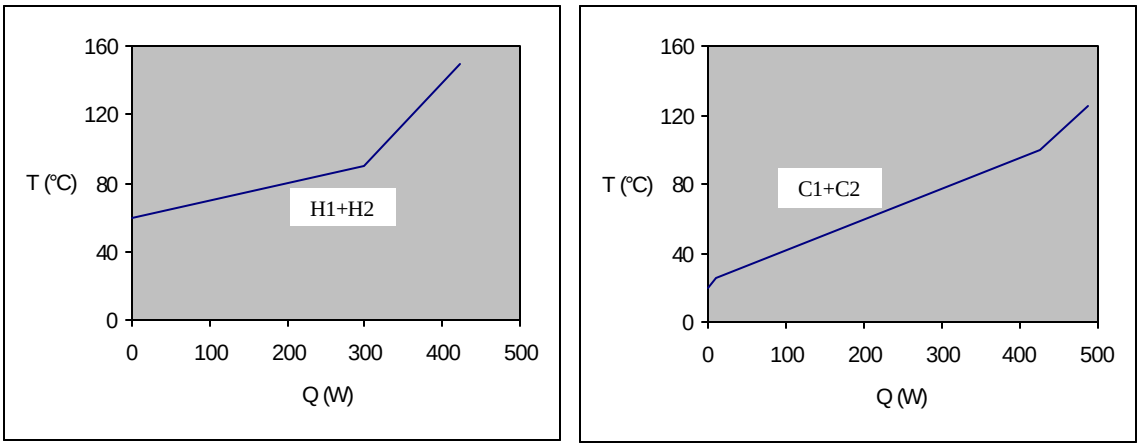


Figure 5. The Composite Curves for Hot Streams (on the left side) and Cold Streams (on the right side) for The Simple Process

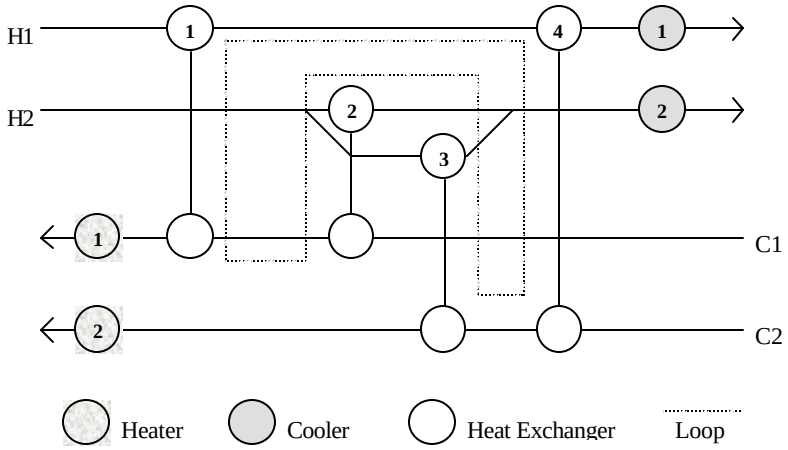


Figure 6. The Grid Diagram

The amount for minimum hot and cold utilities calculated by the Heat Exchanger Network Program is compared with the existing amount of utilities being used in the process. If the existing amounts are greater than the minimum amounts, the process has potential for reduction in operating cost. The network grid diagram synthesized by THEN can be used to construct a heat exchanger network that achieves the target of minimum utilities. The savings in operating costs are compared with the cost of modification of the existing network, and a decision is made about the implementation of the solution proposed by THEN.

The aniline process will be used to demonstrate the use and capabilities of the THEN program. This is described in Section VII.

E. The Pollution Index Program

The final step in the Advanced Process Analysis System is the assessment of the pollution impact of the process on the environment. This has become an important issue in the design and optimization of chemical processes because of growing environmental awareness.

The pollution assessment module of the Advanced Process Analysis System is called 'The Pollution Index Program'. It is based on the Waste Reduction Algorithm (Hilaly, 1994) and the Environmental Impact Theory (Cabezas et. al., 1997).

E-1. Waste Reduction Algorithm

The WAR algorithm is based on the generic pollution balance of a process flow diagram.

Pollution Accumulation = Pollution Inputs + Pollution Generation - Pollution Output (I.1)

It defines a quantity called as the 'Pollution Index' to measure the waste generation in the process. This pollution index is defined as:

$$I = \text{wastes/products} = -(G_{Out} + G_{Fugitive}) / G_{P_n} \quad \text{(I.2)}$$

This index is used to identify streams and parts of processes to be modified. Also, it allows comparison of pollution production of different processes. The WAR algorithm can be used to minimize waste in the design of new processes as well as modification of existing processes.

E-2. The Environmental Impact Theory

The Environmental Impact Theory (Cabezas et. al., 1997) is a generalization of the WAR algorithm. It describes the methodology for evaluating potential environmental impacts, and it can be used in the design and modification of chemical processes. The environmental impacts of a chemical process are generally caused by the energy and material that the process takes from and emits to the environment. The potential environmental impact is a conceptual quantity that can not be measured. But it can be calculated from related measurable quantities.

The generic pollution balance equation of the WAR algorithm is now applied to the conservation of the Potential Environmental Impact in a process. The flow of impact $\dot{I}$, in and out of the process is related to mass and energy flows but is not equivalent to them. The conservation equation can be written as

$$\frac{dI_{sys}}{dt} = \dot{I}_{in} - \dot{I}_{out} + \dot{I}_{gen} \quad \text{(I.3)}$$

where I_{sys} is the potential environmental impact content inside the process, $\dot{I}_{in}$ is the input rate of impact, $\dot{I}_{out}$ is the output rate of impact and $\dot{I}_{gen}$ is the rate of impact generation inside the process by chemical reactions or other means. At steady state, equation I.3 reduces to

$$0 = \dot{I}_{in} - \dot{I}_{out} + \dot{I}_{gen} \tag{I.4}$$

Application of this equation to chemical processes requires an expression that relates the conceptual impact quantity $\dot{I}$ to measurable quantities. The input rate of impact can be written as

$$\dot{I}_{in} = \sum_j \dot{I}_j = \sum_j \dot{M}_j^{in} \sum_k x_{kj} \Psi_k \tag{I.5}$$

where the subscript 'in' stands for input streams. The sum over j is taken over all the input streams. For each input stream j, a sum is taken over all the chemical species present in that stream. M_j is the mass flow rate of the stream j and the x_{kj} is the mass fraction of chemical k in that stream. Ψ_k is the characteristic potential impact of chemical k.

The output streams are further divided into two different types: Product and Non-product. All non-product streams are considered as pollutants with positive potential impact and all product streams are considered to have zero potential impact. The output rate of impact can be written as

$$\dot{I}_{out} = \sum_j \dot{I}_j = \sum_j \dot{M}_j^{out} \sum_k x_{kj} \Psi_k \tag{I.6}$$

where the subscript 'out' stands for non-product streams. The sum over j is taken over all the non-product streams. For each stream j, a sum is taken over all the chemical species.

Knowing the input and output rate of impact from the equations I.5 and I.6, the generation rate can be calculated using equation I.4. Equations I.5 and I.6 need values of potential environmental impacts of chemical species. The potential environmental impact of a chemical species (Ψ_k) is calculated using the following expression

$$\Psi_k = \sum_l \varepsilon_l \Psi^s_{k,l} \tag{I.7}$$

where the sum is taken over the categories of environmental impact. ε_l is the relative weighting factor for impact of type l independent of chemical k. $\Psi^s_{k,l}$ is the potential environmental impact of chemical k for impact of type l. Values of $\Psi^s_{k,l}$ for a number of chemical species can be obtained from the report on environmental life cycle assessment of products (Heijungs, 1992).

There are nine different categories of impact. These can be subdivided into four physical potential impacts (acidification, greenhouse enhancement, ozone depletion and photochemical oxidant formation), three human toxicity effects (air, water and soil) and two ecotoxicity effects (aquatic and terrestrial). The relative weighting factor ε_l allows the above expression for the impact to be customized to specific or local conditions. The suggested procedure is to initially set values of all relative weighting factors to one and then allow the user to vary them according to local needs. More information on impact types and choice of weighting factors can be obtained from the report on environmental life cycle assessment of products (Heijungs, 1992).

To quantitatively describe the pollution impact of a process, the conservation equation is used to define two categories of Impact Indexes. The first category is based on generation of potential impact within the process. These are useful in addressing the questions related to the internal environmental efficiency of the process plant, i.e., the ability of the process to produce desired products while creating a minimum of environmental impact. The second category measures the emission of potential impact by the process. This is a measure of the external environmental efficiency of the process i.e. the ability to produce the desired products while inflicting on the environment a minimum of impact.

Within each of these categories, three types of indexes are defined which can be used for comparison of different processes. In the first category (generation), the three indexes are as follows.

1) $\dot{I}_{gen}^{NP}$ This measures the the total rate at which the process generates potential environmental impact due to nonproducts. This can be calculated by subtracting the input rate of impact ($\dot{I}_{in}$) from the output rate of impact ($\dot{I}_{out}$).Total rate of Impact generated based on Potential Environmemtal Impact is:

$$\dot{I}_{gen}^{NP} = \dot{I}_{in} - \dot{I}_{out} \qquad \text{(I.8)}$$

where $\dot{I}_{in}$ is calculated using equation I.5 and $\dot{I}_{out}$ is calculated using Equation I.6.

2) $\hat{I}_{gen}^{NP}$ This measures the potential impact created by all nonproducts in manufacturing a unit mass of all the products. This can be obtained from dividing $\dot{I}_{gen}^{NP}$ by the rate at which the process outputs products. Specific Impact generated based on Potential Environmental Impact is:

$$\hat{I}_{gen}^{NP} = \frac{\dot{I}_{gen}^{NP}}{\sum_p \dot{P}_p} = \frac{\dot{I}_{out}^{NP} - \dot{I}_{in}^{NP}}{\sum_p \dot{P}_p} \qquad \text{(I.9)}$$

where $\sum_p \dot{P}_p$ is the total rate of output of products.

3) $\hat{M}_{gen}^{NP}$ This is a measure of the mass efficiency of the process, i.e., the ratio of mass converted to an undesirable form to mass converted to a desirable form. This can be calculated from $\hat{I}_{gen}^{NP}$ by assigning a value of 1 to the potential impacts of all non-products.

Rate of Generation of Pollutants per Unit Product is

$$\hat{M}_{gen}^{NP} = \frac{\sum_j \dot{M}_j^{(out)} \sum_k x_{kj}^{NP} - \sum_j \dot{M}_j^{(in)} \sum_k x_{kj}^{NP}}{\sum_p \dot{P}_p} \qquad \text{(I.10)}$$

The indexes in the second category (emission) are as follows.

4) $\dot{I}_{out}^{NP}$ This measures the the total rate at which the process outputs potential environmental impact due to nonproducts. This is calculated using equation I.6.

5) $\hat{I}_{out}^{NP}$ This measures the potential impact emitted in manufacturing a unit mass of all the products. This is obtained from dividing $\dot{I}_{out}^{NP}$ by the rate at which the process outputs products. Specific Impact Emission based on Potential Environmental Impact is:

$$\hat{I}_{out}^{NP} = \frac{\dot{I}_{out}^{NP}}{\sum_p \dot{P}_p} \qquad \text{(I.11)}$$

6) $\hat{M}_{out}^{NP}$ This is the amount of pollutant mass emitted in manufacturing a unit mass of product. This can be calculated from $\hat{I}_{out}^{NP}$ by assigning a value of 1 to the potential impacts of all non-products. Rate of Emission of Pollutants per Unit Product is:

$$\hat{M}_{out}^{NP} = \frac{\sum_j \dot{M}_j^{(out)} \sum_k x_{kj}^{NP}}{\sum_p \dot{P}_p} \qquad \text{(I.12)}$$

Indices 1 and 4 can be used for comparison of different designs on an absolute basis whereas indices 2, 3, 5 and 6 can be used to compare them independent of the plant size. Higher values of indices mean higher pollution impact and suggest that the plant design is inefficient from environmental safety point of view.

E-3. Steps in Using the Pollution Index Program

The first step in performing pollution analysis is the selection of relevant streams. Environmental impact of a chemical process is caused by the streams that the process takes from and emits to the environment. Therefore, only these input and output streams are considered in performing the pollution index analysis. Other streams, which are completely internal to the process, are excluded. In the Pollution Index Program, this selection of input-output streams is automatically done based on the plant information entered in Flowsim.

The next step in the pollution index analysis is the classification of the output streams into product and non-product streams. All streams which are either sold as product or which are used up in a subsequent process in the production facility are considered as product streams. All other output streams, which are released into the environment, are considered as non-product streams. All non-product streams are considered as pollutant streams whereas all product streams are considered to have zero environmental impact.

Pollution index of a stream is a function of its composition. The composition data for the streams is retrieved from the results of on-line optimization performed earlier. This can be either in terms of the molar flowrates or fractions. Additional data such as the specific environmental impact potential values for the chemical species is available in the report on environmental life cycle assessment of products.

The last piece of information required is the relative weighting factors for the process plant. These values depend on the location of the plant and its surrounding conditions. For example, the weighting factor for photochemical oxidation is higher in areas that suffer from smog.

Having finished all of the above prerequisite steps, the pollution index program is now called to perform the analysis. Mass balance constraints are solved for the process streams involved, and the equations of the Environmental Impact Theory are used to calculate the pollution index values. The pollution indices of the six types discussed earlier are reported for the process. Three of these are based on internal environmental efficiency whereas the other three are based on external environmental efficiency. Higher the values of these indices, higher the environmental impact of the process.

The pollution index program also calculates pollution indices for each of the individual process streams. These values help in identification of the streams that contribute more to the overall pollution impact of the process. Suitable process modifications can be done to reduce the pollutant content of these streams.

Every run of on-line optimization for the process is followed by the pollution index calculations. The new pollution index values are compared with the older values. The comparison shows how the change in process conditions affects the environmental impact. Thus, the pollution index program can be used in continuous on-line monitoring of the process.

The aniline process will be used to demonstrate the use and capabilities of the pollution index program. This is described in Section VIII.

F. Windows Interface

An important part of the advanced process analysis system is development of the Graphical User Interface (GUI). It was necessary to have a programming language, which could integrate all of above applications into one program. It should also be able to exchange information between these programs without the intervention of the process engineer.

There are four competitive object-oriented, rapid applications development tools with GUI windows that have the above capabilities. These are Microsoft's Visual Basic, Borland's Delphi32, IBM's Visual Age and Powersoft's Powerbuilder.

We have chosen Visual Basic as the interface development language. It is integrated with Windows 95/98 and Windows NT, has a low cost and can link applications over a local area network. Also, Visual Basic supports the Object Linking and Embedding technology in OLE2. This feature allows the programs to exchange information regardless of the physical or logical location or data type and format.

Visual Basic 5.0 was used to develop windows interface for Flowsim, the on-line optimization program, the chemical reactor design program, THEN, the heat exchanger network design program, and the pollution index program. As mentioned earlier, sharing of process, economic and environmental data is the key to integration of these programs into one package. Storing the output data of all these programs in different files had many disadvantages. Both storage and retrieval of data would be inefficient. Also, exchange of information between the programs would require reading data from a number of files thus reducing the speed.

As a result, it was decided to use a database to store all of the necessary information to be shared by the component programs as shown in Figure 1. A database is nothing but a collection of information in form of tables. The information in a table is related to a particular subject or purpose. A number of database formats are in use in industry. We have chosen Microsoft Access as the database system for this project.

A table in Microsoft Access consists of rows and columns, which are called *Records* and *Fields* respectively in the database terminology. Each *Field* can store information of a particular kind e.g. a table 'Stream Data' can have a field called 'Temperature' which stores all the stream temperatures. Another table can have a field called 'Prices' which has the prices of all the reactants and products. Each *Record* is a data entry, which fills all the fields of a table. So, the Stream Data table in the above example can have a record for stream S1, which has values for temperatures, pressure, flowrates etc. entered in the respective fields.

Microsoft Access is an interactive database system. Using Access, you can store data in tables according to the subject. This makes tracking of data very efficient. Also, you can specify relationships between different tables. Consequently, it is easy to bring together information related to various topics. Microsoft Access takes full advantage of the graphical power of windows. Also, it is fully compatible with Microsoft's Visual Basic and Microsoft Excel, which is a significant advantage for this application.

G. Summary

The Advanced Process Analysis System offers a combination of powerful process design and modification tools. The Visual Basic interface integrates all of these into one system and makes the application very user-friendly. The best way to understand the application of the Advanced Process Analysis System is to apply it to a relatively simple plant. The simulation of the aniline process has been selected as the example process. This process incorporates nearly all of the process units found in chemical plant and refineries including packed bed catalytic chemical reactors, distillation columns and heat exchangers among others. The next section gives a detailed description of the simulation of the aniline process. The contact process for sulfuric acid manufacture process (D-train) at IMC Agrico, Convent, Louisiana is described in a separate manual.

II. EXAMPLE - ANILINE PROCESS DESCRIPTION

The aniline plant is a simulation of a 55,000 metric tons/yr process for ammonolysis of phenol. The desired yield of aniline in the process is 95% based on phenol and 80% based on ammonia.

The aniline plant uses a three-step process that produces aniline, diphenylamine and water from phenol and ammonia. The process flow diagrams are shown in Figures 7 and 8, and the process consist of the following three sections: the feed preparation section, the reactor section, and the purification section.

In the feed preparation section, the ammonia and phenol feed streams are combined with the ammonia and phenol recycle streams and heated to the required reactor temperature. The ammonia feed stream (stream 1) consists of 203 lb-mol/hr liquid ammonia at 90^{o}F. The phenol feed stream (stream 2) supplies 165.8 lb-mol/hr liquid phenol at 110^{o}F and atmospheric pressure. The two feed streams are pumped to a pressure of 255 psia before they are mixed with their respective recycle streams (stream 16 for ammonia and stream 31 for phenol) forming streams 5 and 6. In addition to ammonia, the ammonia recycle has small amounts of hydrogen, nitrogen and water. The phenol recycle stream consists of phenol, aniline and diphenylamine. Streams 5 and 6 are then mixed together (MIX-102) forming stream 7. Stream 7 is at a temperature of 156^{o}F and at a pressure of 255 psia. The ratio of ammonia to phenol in stream 7 is 20:1. This stream is heated in a cross exchanger (E-100) with the reactor effluent (stream 10). The exchanger has an approach temperature between stream 10 and stream 8 of 75^{o}F along with a pressure drop of 5 psia. Stream 8 emerges at 650^{o}F and 250 psia. The reactor inlet (stream 9) needs to be at 710^{o}F and 245 psia, so stream 8 passes through a heater (E-101).

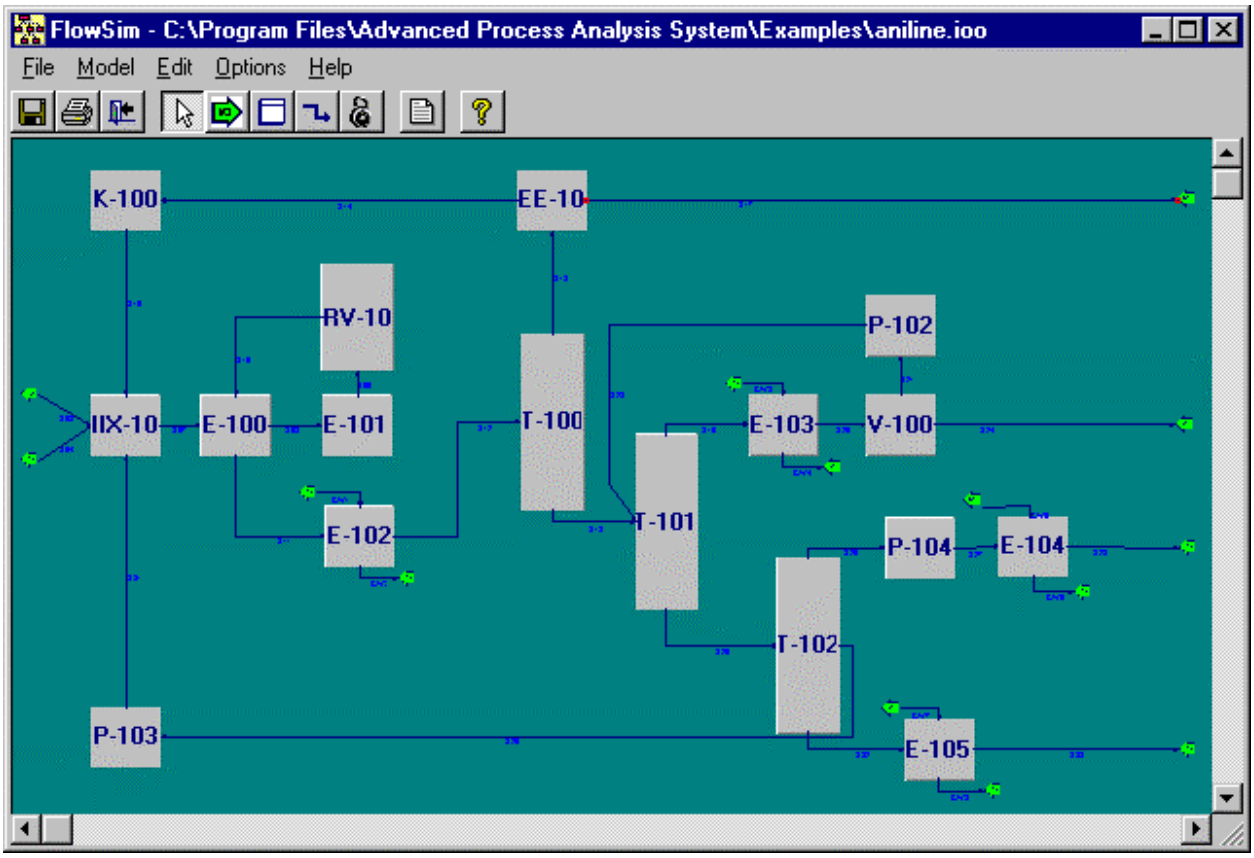


Figure 7: Process Flow Diagram Aniline Process

The reactor section includes the adiabatic reactor (CRV-100) that consists of a bed packed with a silica-alumina catalyst. In the reactor, three reactions occur.

Phenol + NH_3 ➔ Aniline + H_2O

2 Phenol + NH_3 ➔ Diphenylamine + 2 H_2O

2 NH_3 <==> 3 H_2 + N_2

The conversion of phenol in the reactor is 95% with a 99% selectivity to aniline as shown in the first reaction. The second reaction forms another salable product in diphenylamine, while the third reaction is the decomposition of ammonia. The reaction set is slightly exothermic, so the stream leaving the reactor (stream 10) is slightly hotter than stream 9. Also, there is a 5 psia pressure drop across the reactor. Therefore, stream 10 has the following conditions: 725^{o}F and 240 psia.

The cooling of the reactor effluent begins with the cross exchanger (E-100) which cools stream 10 by about 500^{o}F. Again there is a 5 psia pressure drop across the cross exchanger. Stream 11 is at a temperature of 223^{o}F and a pressure of 235 psia. Finally, stream 11 is sent through a cooler (E-102). Every cooler has a stream of water passing through it to cool the process stream. The water enters at 80^{o}F and leaves at 100^{o}F. For this cooler, the approach

temperature between the water inlet (CW1) and stream 12 is 60°F and the pressure drop is 5 psia. Thus, stream 12 is at 140°F and 230 psia.

The purification section consists of the distillation columns to separate the chemicals into products and non-products. The absorption column (T-100) separates the gases and the liquids. T-100 is a 10-stage reboiled absorber (no condenser) fed at the top stage. The pressure at the top of the column is 220 psia, while the pressure at the bottom of the column is 222.5 psia. The light key component of this column is ammonia, while the heavy key component is water. Theory says that any component lighter than the light key will appear in the distillate. Therefore, all of the hydrogen and nitrogen go to stream 13. Theory also suggests that any component heavier than the heavy key will appear in the bottoms product. Thus, all of the phenol, aniline and diphenylamine go to stream 18. As for the key components, 99.9% of the ammonia and 10% of the water go to the distillate.

From the absorption column, stream 13 goes to a splitter. The splitter sends 98.9% of the stream to stream 14, which is the ammonia recycle stream. Since the recycle stream is not at the same pressure as stream 3, it is passed through a compressor. Stream 16 emerges at 170°F and 255 psia. The splitter also sends 1.1% of stream 13 to the gaseous purge, stream 17. The purge is necessary to avoid any pressure build-up in the process. Stream 17 is a non-product stream, but it is used as fuel for the heater. The bottoms stream (stream 18) is one of the feeds to the next column.

The second column in the purification section is the drying column (T-101). The column has 25 stages and is fed at the top stage by streams 18 and 23. The pressure at the top of the column is 15 psia, and the pressure at the bottom of the column stage is 21.25 psia. The key components are water and phenol. However, some aniline is lost in the distillate because aniline is soluble in water. The distillate contains 99.99% of the water, 6% of the phenol and 5% of the aniline fed to the column (streams 18 and 23). The distillate, stream 19, is cooled by E-103 to a temperature of 110°F with a pressure of 10 psia. Stream 20 is then sent to a three-phase separator (V-100) to separate the aqueous product and the liquid (organic) product. The organic product (stream 21) is recycled to the column. Stream 21 consists of 7% of the ammonia, 3% of the water, 30.5% of the phenol and 86% of the aniline in stream 20. Because stream 21 is below the pressure of the top stage pressure, P-102 is used to bring the pressure in stream 23 up to 15 psia. The aqueous product (stream 24) from V-100 is a non-product output stream. This stream will be sent through wastewater treatment and released off-site. The bottoms stream (stream 25) is the feed to the next column.

The final column is the product column (T-102). It is a 75-stage column fed on stage 35. The pressure at the top of the column is 2.707 psia, while the pressure at the bottom of the column is 21.46 psia. This column also has a side draw on stage 50. Due to a high-boiling azeotrope between phenol and aniline, the main component in the distillate (stream 26) is aniline. Stream 26 contains all of the water, 19.5% of the phenol and 92.3% of the aniline from stream 25. Stream 26 must be at least 99 wt% aniline for industrial use. Because there is a 10 psia pressure drop for liquids in coolers, stream 26 needs to be pumped up to a pressure of 12.71 psia by P-104. The resulting stream (stream 27) is cooled by E-104. Stream 28, a product stream, emerges from the cooler at 90°F and 2.707 psia. The azeotrope between phenol and aniline is

taken off on stage 50 and recycled. This azeotrope (stream 29) contains 33 wt% phenol, 65 wt% aniline and 2 wt% diphenylamine. These weight percents account for 80% of the phenol, 7.7% of the aniline and 4.6% of the diphenylamine in stream 25. Stream 29 is below the pressure of stream 4, therefore it is pumped to a pressure of 255 psia by P-103. Stream 31 emerges at 373^{o}F and 255 psia. The bottoms product (stream 32) consists of 5% of the phenol and 95.4% of the diphenylamine in stream 25. Stream 32 must be at least 95 wt% diphenylamine for industrial use. This stream is then cooled by E-105. Stream 33, a product stream, emerges from E-105 at 130^{o}F and 11.46 psia.

This concludes the description of the aniline process. The next section explains the development of the process model.

III. PROCESS MODEL FOR THE ANILINE PROCESS

A process model of a chemical engineering process is a set of constraint equations, which represents a mathematical model of relationships between the various plant units and process streams. Before the constraint equations are formulated, it is important to note that in order to have an accurate model of the process, it is essential to include the key process units such as reactors, heat exchangers and absorbers. These units affect the economic and pollution performance of the process to a significant extent. Certain other units are not so important and can be excluded from the model without compromising the accuracy. For the aniline process, the five heat exchangers, the three distillation columns, three of the five pumps, the reactor, the compressor, the splitter and the three-phase separator were identified as the important units to be included in the model whereas the two feed pumps were excluded from the model. The process model diagram with these units and streams is shown in Figure 8. The complete list of the process units and process streams included in the model is given in Tables 1 and 2.

Having selected the process units and streams, the next step is to develop the constraint equations. The constraint equations are entered in Flowsim using the format of the GAMS language. They become the process model which is used to reconcile plant measurements, estimate parameters, optimize the profit and minimize emissions from the plant. The constraint formulation techniques are very similar for process units of the same type. Therefore, this section is divided into four sub-sections; heat exchanger network, reactors, absorption towers and overall balance for the plant. Each of these sub-sections explains how constraints (material and energy balances) are written for that particular type of unit. For each type, detailed constraint equations are shown for a representative unit.

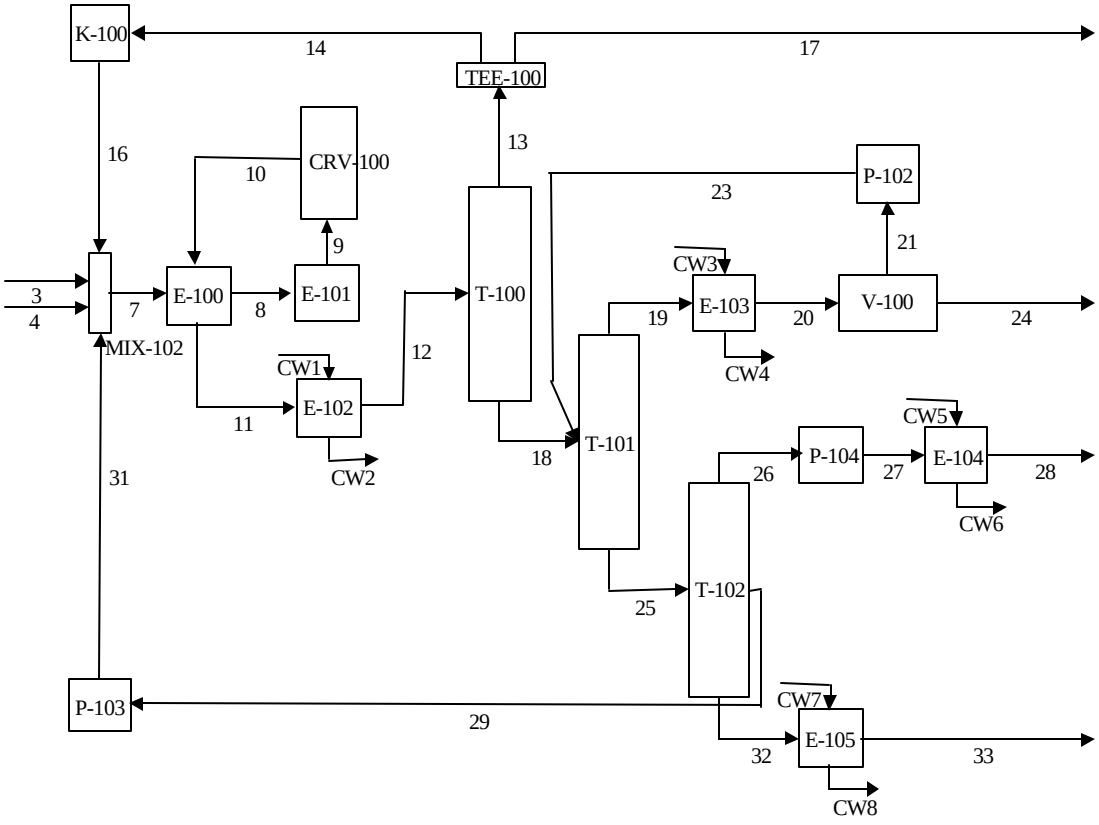


Figure 8. The Process Model Diagram for Aniline Process.

Table 1 Process Units for the Aniline Process Model (Refer to Figure 8, the Process Model Diagram)

Name of Unit	**Description**
MIX-102	Feed and recycle mixer
E-100	Cross heat exchanger
E-101	Process heater
CRV-100	Reactor
E-102	Reactor product cooler
T-100	Absorption tower
TEE-100	Purge/recycle splitter
K-100	Ammonia recycle compressor
T-101	Drying column
E-102	Drying column condenser
V-100	Three-phase separator
P-102	Separator recycle pump
T-102	Product column
P-104	Aniline product pump
E-104	Aniline product cooler
P-103	Phenol recycle pump
E-105	DPA product cooler

Table 2 Process Streams in the Aniline Process Model (Refer to Figure 8, the Process Model Diagram)

Name of Stream	Description
s03	Ammonia feed
s04	Phenol feed
s07	Mixed stream
s08	Heater feed
s09	Reactor feed
s10	Reactor effluent
s11	Cooler feed
s12	T-100 feed
s13	T-100 overhead
s14	Ammonia recycle
s16	High pressure ammonia recycle
s17	Gaseous purge
s18	T-101 feed
s19	T-101 overhead
s20	Separator feed
s21	Separator recycle
s23	High pressure separator recycle
s24	Water product
s25	T-102 feed
s26	T-102 overhead
s27	High pressure aniline product
s28	Aniline product
s29	Phenol recycle
s31	High pressure phenol recycle
s32	T-102 bottoms
s33	DPA product
CW1	Cooling water to reactor product cooler
CW2	Cooling water from reactor product cooler
CW3	Cooling water to drying column condenser
CW4	Cooling water from drying column condenser
CW5	Cooling water to aniline product cooler
CW6	Cooling water from aniline product cooler
CW7	Cooling water to DPA product cooler
CW8	Cooling water from DPA product cooler

A. Heat Exchanger Network

As shown in Figure 8, the heat exchanger network in the aniline process includes the cross heat exchanger (E-100), the heater (E-101), and the product cooler (E-102). The inlet component flowrates are equal to the outlet component flow rates for both sides. The energy balance states that the decrease of the enthalpy (10^6 Btu/hr) in the hot side is equal to the increase of enthalpy in cold side plus the heat loss, i.e.,

$$(H^{inlet} - H^{outlet})_{hot} = (H^{outlet} - H^{inlet})_{cold} + Q_{loss}. \qquad \text{(III.1)}$$

For the cross heat exchanger (E-100), s07s the inlet stream on the cold side whereas s08 is the outlet stream on the cold side. s10 is the inlet stream on the cold side and s11 is the outlet stream on hot side. The energy balance can be written as

$$(H^{inlet} - H^{outlet})_{cold} = G\, f_{07}^{(i)} h_{07}^{(i)} - G\, f_{08}^{(i)} h_{08}^{(i)} \quad \text{and} \qquad \text{(III.2)}$$
$$(H^{inlet} - H^{outlet})_{hot} = G\, f_{10}^{(i)} h_{10}^{(i)} - G\, f_{11}^{(i)} h_{11}^{(i)}$$

where $f_{07}^{(i)}$ is the molar flowrate (lb-mol/hr) of species i in stream s07 and $h_{07}^{(i)}$ is the enthalpy (10^6 Btu/lb-mol) of species i in stream s07. The total molar flowrate of stream s07 and the total enthalpy of stream s07 are given by the equations

$$f_{07} = G\, f_{07}^{(i)} \quad \text{and} \qquad \text{(III.3)}$$
$$H_{07} = G\, f_{07}^{(i)} h_{07}^{(i)}$$

where the summation is done over all the species i present in stream s07. This naming convention is used for all the flowrates and enthalpies. The number in the subscript of the variable can be used to identify the stream to which it belongs. H^{inlet}_{cold} is the enthalpy of the inlet stream on the cold side, and it has units of 10^6 Btu/hr.

The heat transferred in an exchanger is proportional to heat transfer area A, overall heat transfer coefficient U, and the logarithmic mean temperature difference between the two sides ΔT_{lm}, i.e., $Q = UA\,\Delta T_{lm}$, where Q is the enthalpy change on the cold side, i.e.,

$$Q = (H^{inlet} - H^{outlet})_{cold} = G\, f_{07}^{(i)} h_{07}^{(i)} - G\, f_{08}^{(i)} h_{08}^{(i)} \qquad \text{(III.4)}$$

The material and energy balances as well as the heat transfer equations are similar for all units in the heat exchanger network. Table 3 gives the constraint equations for the cross heat exchanger as an example of process constraint equations for all heat exchanger units.

The first two rows of the Table 3 under material balance give the overall mass balance and all of the species mass balances. The overall mass balance is the summation of all species mass balances. Therefore, if all of the species mass balances are used to describe the process, then the overall mass balance does not need to be included since it is redundant. The species mass balances are used to describe the relationship of the input and output flow rate variables.

Table 3 The Constraint Equations for the Cross Heat Exchanger(E-100)

Material Balances	
Overall	$(f_{08}^{(H_2)} + f_{08}^{(N_2)} + f_{08}^{(NH_3)} + f_{08}^{(H_2O)} + f_{08}^{(PH)} + f_{08}^{(AN)} + f_{08}^{(DPA)}) -$ $(f_{07}^{(H_2)} + f_{07}^{(N_2)} + f_{07}^{(NH_3)} + f_{07}^{(H_2O)} + f_{07}^{(PH)} + f_{07}^{(AN)} + f_{07}^{(DPA)}) = 0$ $(f_{11}^{(H_2)} + f_{11}^{(N_2)} + f_{11}^{(NH_3)} + f_{11}^{(H_2O)} + f_{11}^{(PH)} + f_{11}^{(AN)} + f_{11}^{(DPA)}) -$ $(f_{10}^{(H_2)} + f_{10}^{(N_2)} + f_{10}^{(NH_3)} + f_{10}^{(H_2O)} + f_{10}^{(PH)} + f_{10}^{(AN)} + f_{10}^{(DPA)}) = 0$
Species	H_2: $f_{08}^{(H_2)} - f_{07}^{(H_2)} = 0$, $f_{11}^{(H_2)} - f_{10}^{(H_2)} = 0$ N_2: $f_{08}^{(N_2)} - f_{07}^{(N_2)} = 0$, $f_{11}^{(N_2)} - f_{10}^{(N_2)} = 0$ NH_3: $f_{08}^{(NH_3)} - f_{07}^{(NH_3)} = 0$, $f_{11}^{(NH_3)} - f_{10}^{(NH_3)} = 0$ H_2O: $f_{08}^{(H_2O)} - f_{07}^{(H_2O)} = 0$, $f_{11}^{(H_2O)} - f_{10}^{(H_2O)} = 0$ PH: $f_{08}^{(PH)} - f_{07}^{(PH)} = 0$, $f_{11}^{(PH)} - f_{10}^{(PH)} = 0$ AN: $f_{08}^{(AN)} - f_{07}^{(AN)} = 0$, $f_{11}^{(AN)} - f_{10}^{(AN)} = 0$ DPA: $f_{08}^{(DPA)} - f_{07}^{(DPA)} = 0$, $f_{11}^{(DPA)} - f_{10}^{(DPA)} = 0$
Energy Balances	
Overall	$\left(\sum_i F_{14}^{(i)} h_{14}^{(i)} \& \sum_i F_{13}^{(i)} h_{13}^{(i)}\right) \& \left(\sum_i F_{19}^{(i)} h_{19}^{(i)} \& \sum_i F_{20}^{(i)} h_{20}^{(i)}\right) \% Q_{loss} ' 0$ where $h^i{}_k(T) ' R(a_1^i T \% \frac{1}{2} a_2^i T^2 \% \frac{1}{3} a_3^i T^3 \% \frac{1}{4} a_4^i T^4 \% \frac{1}{5} a_5^i T^5 \% b_1^i \& H_{298}^i)$ $i ' SO_2, SO_3, O_2, N_2;\ k ' 13, 14, 19, 20$
Heat Transfer	$\left(\sum_i F_{20}^{(i)} h_{20}^{(i)} \& \sum_i F_{19}^{(i)} h_{19}^{(i)}\right) \& (U_{ex66} A_{ex66}) T_{lm}) ' 0$

In the constraints of Table 3, f denotes the component molar flow rate, lb-mol/hr, and its superscript i and subscript k denote the component names and stream numbers respectively. h's in the equations represent the species enthalpies of streams (10^6 Btu/lb-mol), and Q_{loss} is the heat loss from the exchanger (10^6 Btu/lb-mol). T is the stream temperature (^oR), and ΔT_{lm} is the logarithmic mean temperature difference (^oR) between hot and cold sides of the exchanger. In the heat transfer equation, U and A are the overall heat transfer coefficient and heat transfer area respectively.

The two rows in Table 3 under energy balances give the overall energy balance and heat transfer equation. In addition, the enthalpy for each species, h(T), expressed as a polynomial function of the stream temperature is also given in the table. The enthalpy equations for gases and liquids follow Equation III.5 .

$$\left(\sum_i f_{10}^{(i)} h_{10}^{(i)} - \sum_i f_{11}^{(i)} h_{11}^{(i)}\right) - \left(\sum_i f_{08}^{(i)} h_{08}^{(i)} - \sum_i f_{07}^{(i)} h_{07}^{(i)}\right) + Q_{loss} = 0 \qquad \text{(III.5)}$$

where

$$h_k^{(i)}(T) = a_1^{(i)} T + a_2^{(i)} T^2 + a_3^{(i)} T^3 + a_4^{(i)} T^4$$

$$i = H_2, N_2, NH_3, H_2O, PH, AN, DPA$$

Table 4 shows the enthalpy coefficients (a_1, a_2, a_3 and a_4) for gases and liquids.

In these equations, the total flow rates, species flow rates (or composition), and temperatures of streams are the measurable variables. Species enthalpies and the mean temperature difference are also measurable variables because they can be calculated from other measurable variables such as temperatures and flowrates. The heat transfer coefficients are the process parameters to be estimated. The heat transfer area, heat loss and coefficients in enthalpy equations are constants. The heat loss is 0 for this simulation. The equations for the other heat exchangers are shown in Appendix A.

B. Reactor System

The reactor system in this plant includes a fixed bed catalytic reactor The following describes the constraint equations for reactor.

When a chemical reaction is involved in the process, it is convenient to use the mole balance to describe relationship of input and output flow rates of a unit for each component. Also, the overall mole balance is obtained from the component mole balances, i.e., the summation of component mole balances gives the overall mole balance. The aniline process involves three reactions, i.e., The formation aniline, the formation of diphenylamine and the the decomposition of ammonia. Mole balances are used to describe the material balances of the units in the process, i.e., all material balance equations for the aniline process are written with mole balance relations. Moles are conserved when there is no reaction, and the change in the number of moles for a component is determined by the reaction rate and stoichiometric coefficients when there are reactions.

Table 4. Enthalpy Coefficients for Gases and Liquids.

Gases				
	a_1	a_2	a_3	a_4
H_2	6.7762	1.2745E-04	-3.1784E-08	1.2545E-11
N_2	6.9872	-1.9897E-04	2.2049E-07	-3.4903E-11
NH_3	6.5140	1.7334E-03	2.4376E-07	-6.9535E-11
H_2O	7.8055	-4.7750E-05	3.4883E-07	-5.0150E-11
Phenol	-3.4274	3.1755E-02	-7.2633E-06	6.7130E-10
Aniline	-2.8491	3.3895E-02	-8.0960E-06	8.1465E-10
Diphenylamine	-19.242	7.0815E-02	-1.8014E-05	1.9146E-09
Liquids				
NH_3	-43.507	2.2304E-01	-3.5380E-04	2.0857E-07
H_2O	21.986	-2.6508E-03	-5.1857E-06	5.4745E-09
Phenol	9.2247	7.2870E-02	-6.1180E-05	2.3346E-08
Aniline	15.116	6.5655E-02	-5.7950E-05	2.3852E-08
Diphenylamine	17.304	9.6945E-02	-7.2647E-05	2.4965E-08

As shown in Figure 8, the input to the reactor is a stream (s09) mixed with all the components at the design operating temperature (710^{o}F) and pressure (245 psia). One molecule phenol reacts with one molecule of ammonia to produce aniline, but a side reaction causes two molecules of phenol to react with one molecule of ammonia to produce diphenylamine. Another side reaction causes ammonia to decompose into hydrogen and nitrogen. Research has shown that the selectivity of the phenol and ammonia reactions to aniline is 99%, while less than 1% of the ammonia decomposes to hydrogen and nitrogen. These values are incorporated in the mass and energy balances of this unit.

The mole and energy balance equations for the reactor are given in Table 5. The two rows of this table under mole balance give the overall mole balance and component mole balances. The mole balance for each component is established based on the conservation law. The steady state mole balance for a component is written as:

$$F_{in}(i) - F_{out}(i) + F_{gen}(i) = 0 \qquad \text{(III.6)}$$

where i represents the names of components. For the sulfur burner, $F_{in}(i)$, $F_{out}(i)$, and $F_{gen}(i)$ are input air flow rate F06(i), output flow rate F07(i), and generation rates of components from reaction, r(i). The overall mole balance is the summation of all component mole balance equations.

Three reactions take place in this unit, i.e., reaction one of phenol and ammonia to aniline and water, reaction two of phenol and ammonia to diphenylamine and water and reaction three of ammonia to hydrogen and nitrogen. The first two reactions are based on the conversion of phenol and the selectivity of the reaction. The conversion of phenol in the reactor is 95%, while the selectivity is 99% to aniline. Therefore, the reaction (generation) rate for phenol, ammonia, aniline, diphenylamine and water is related to the input flow rate of phenol, f_{09}^{PH}, and the stoichiometric coefficient of the component in the reaction. Also, the reaction rate of a product component has a positive value and the reaction rate of a reactant component has a negative value. For example, the component mole balance for aniline is:

$$\text{AN:} \qquad f_{10}^{(AN)} - f_{09}^{(AN)} - 0.99 * conv1 * f_{09}^{(PH)} = 0 \qquad \text{(III.7)}$$

where $f_{09}^{(AN)}$ and $f_{10}^{(AN)}$ are the input and output flow rates of aniline, and $0.99 * conv1 * f_{09}^{(PH)}$ is the generation rate of sulfur dioxide. The variable $conv1$ is the conversion of phenol in the reactor; it is treated as a parameter since the conversion can vary based on the life of the catalyst.

The steady state overall energy balance is established based on the first law of thermodynamics. Neglecting changes in kinetic and potential energy, this equation is (Felder and Rousseau, 1986):

$$f_{in}(i)h_{in}(i) - f_{out}(i)h_{out}(i) + Q - W = 0 \qquad \text{(III.8)}$$

where i represents the components entering and exiting the reactor. Since the reactor is an adiabatic reactor, Q = 0. No work is done on or by the reactor, thus W = 0. These assumptions lead to the following energy balance on the reactor:

$$f_{in}(i)h_{in}(i) - f_{out}(i)h_{out}(i) = 0 \qquad \text{(III.9)}$$

In Table 5, f denotes stream species flow rate, lb-mol/sec, and h represents species enthalpy, 10^6 Btu/lb-mol. The detailed enthalpy regression functions for all components are given in Appendix A.

The reactor in the aniline plant is an adiabatic, plug flow reactor that converts phenol and ammonia to aniline and water in an exothermic chemical reaction. Along with this reaction, there are two side reactions that occur in the reactor. The kinetic model for the aniline reaction was formulated by using data from patents and making a pseudo-first order assumption for the formation of aniline. Below are the kinetic equations for the process where the constants have units consistent with the units in the Reactor Analysis program.

$$\begin{aligned} r_1 &= 0.0191887 * c_{PH} \\ r_2 &= 9.69127E-05 * c_{PH} \\ r_3 &= 2.4E14 * \exp[-59784/T] * c_{NH_3}{}^2 \end{aligned} \qquad \text{(III.10)}$$

Table 5. The Process Constraint Equations for the Reactor (CRV-100)

Material Balances	
Overall	$f_{09} = f_{09}^{(H_2)} + f_{09}^{(N_2)} + f_{09}^{(NH_3)} + f_{09}^{(H_2O)} + f_{09}^{(PH)} + f_{09}^{(AN)} + f_{09}^{(DPA)}$ $f_{10} = f_{10}^{(H_2)} + f_{10}^{(N_2)} + f_{10}^{(NH_3)} + f_{10}^{(H_2O)} + f_{10}^{(PH)} + f_{10}^{(AN)} + f_{10}^{(DPA)}$ $feedconc = \sum_i feed\_i \quad effconc = \sum_i eff\_i$ $i = H_2, N_2, NH_3, H_2O, PH, AN, DPA$
Species	H_2: $f_{10}^{(H_2)} - f_{09}^{(H_2)} - 1.5 * conv2 * f_{09}^{(NH_3)} = 0$ N_2: $f_{10}^{(N_2)} - f_{09}^{(N_2)} - 0.5 * conv2 * f_{09}^{(NH_3)} = 0$ NH_3: $f_{10}^{(NH_3)} - (1 - conv2) f_{09}^{(NH_3)} - 0.995 * conv1 * f_{09}^{(PH)} = 0$ H_2O: $f_{10}^{(H_2O)} - f_{09}^{(H_2O)} - conv1 * f_{09}^{(PH)} = 0$ PH: $f_{10}^{(PH)} - (1 - conv1) * f_{09}^{(PH)} = 0$ AN: $f_{10}^{(AN)} - f_{09}^{(AN)} - 0.99 * conv1 * f_{09}^{(PH)} = 0$ DPA: $f_{10}^{(DPA)} - f_{09}^{(DPA)} - 0.05 * conv1 * f_{09}^{(PH)} = 0$ $feed\_i = \frac{1000 * f_{09}^{(i)} * density_{(i)}}{f_{09} * MW_{(i)}} \quad eff\_i = \frac{1000 * f_{10}^{(i)} * density_{(i)}}{f_{10} * MW_{(i)}}$ $i = H_2, N_2, NH_3, H_2O, PH, AN, DPA$
Energy Balances	
Overall	$\sum_i f_{10}^{(i)} h_{10}^{(i)} - \sum_i f_{09}^{(i)} h_{09}^{(i)} + Q_{loss} = 0$
Enthalpy Function	$h_k^{(i)}(T) = a_1^{(i)} T + a_2^{(i)} T^2 + a_3^{(i)} T^3 + a_4^{(i)} T^4$ $i = H_2, N_2, NH_3, H_2O, PH, AN, DPA; \quad k = 10,11$ s09: all chemicals use gaseous enthalpy coefficients s10: all chemicals use gaseous enthalpy coefficients

C. Absorber Tower Section

This section includes the absorption tower, the drying column and the product column. These units involve the separation of aniline and diphenylamine from the other, non-scalable reactor products. In Table 6, the material balance equations are given for the absorption tower and the drying column.

In Table 6, the first tow rows give the total and component mole balances for the absorption tower whereas the next row gives the energy balance function for the streams associated with the absorption tower.

D. Overall Material Balance

The overall material balance relates the flow rates of raw materials to the production of products and wastes. The overall material balance also creates some constraints over the system. There are five constraints of this system. The first constraint for the process is the molar ratio of ammonia and phenol in stream 7:

$$f_{07}^{(NH_3)} / f_{07}^{(PH)} \geq 17 \qquad \text{(III.11)}$$

The second and constraint is the necessary weight fraction of aniline in the product stream:

$$x_{26}^{(AN)} \geq 0.99 \qquad \text{(III.12)}$$

where $x_{26}^{(AN)}$ is the weight fraction of aniline. The third and fourth constraints are the necessary weight fractions of phenol and aniline in the phenol recycle stream:

$$x_{29}^{(PH)} \geq 0.30 \qquad \text{(III.13)}$$

$$x_{29}^{(AN)} \geq 0.65 \qquad \text{(III.14)}$$

where $x_{29}^{(PH)}$ and $x_{29}^{(AN)}$ are the weight fractions of phenol and aniline, respectively. The final constraint is the necessary weight fraction of diphenylamine in the DPA product:

$$x_{26}^{(DPA)} \geq 0.945 \qquad \text{(III.15)}$$

where $x_{26}^{(DPA)}$ is the weight fraction of diphenylamine.

This concludes the discussion of model formulation for the aniline process. Having understood the methodology of Advanced Process Analysis System and the aniline process model, we are now ready to use the Advanced Process Analysis System program. The following section gives detailed instructions on using the program.

Table 6. The Constraint Equations for the Absorption Tower (T-100)

Material Balances	
Overall	$(f_{13}^{(H_2)} + f_{13}^{(N_2)} + f_{13}^{(NH_3)} + f_{13}^{(H_2O)}) +$ $(f_{18}^{(NH_3)} + f_{18}^{(H_2O)} + f_{18}^{(PH)} + f_{18}^{(AN)} + f_{18}^{(DPA)}) -$ $(f_{12}^{(H_2)} + f_{12}^{(N_2)} + f_{12}^{(NH_3)} + f_{12}^{(H_2O)} + f_{12}^{(PH)} + f_{12}^{(AN)} + f_{12}^{(DPA)}) = 0$
Species	H_2: $f_{13}^{(H_2)} - f_{12}^{(H_2)} = 0$ N_2: $f_{13}^{(N_2)} - f_{12}^{(N_2)} = 0$ NH_3: $f_{13}^{(NH_3)} - 0.999 f_{12}^{(NH_3)} = 0$ $f_{18}^{(NH_3)} - 0.001 f_{12}^{(NH_3)} = 0$ H_2O: $f_{13}^{(H_2O)} - 0.10 f_{12}^{(H_2O)} = 0$ $f_{18}^{(H_2O)} - 0.90 f_{12}^{(H_2O)} = 0$ PH: $f_{18}^{(PH)} - f_{12}^{(PH)} = 0$ AN: $f_{18}^{(AN)} - f_{12}^{(AN)} = 0$ DPA: $f_{18}^{(DPA)} - f_{12}^{(DPA)} = 0$
Energy Balances	
Enthalpy Function	$h_k^{(i)}(T) = a_1^{(i)}T + a_2^{(i)}T^2 + a_3^{(i)}T^3 + a_4^{(i)}T^4$ $i = H_2, N_2, NH_3, H_2O, PH, AN, DPA$; $k = 13,18$ s13: all chemicals use gaseous enthalpy coefficients s18: all chemicals use gaseous enthalpy coefficients

IV. GETTING STARTED WITH THE ADVANCED PROCESS ANALYSIS SYSTEM

Upon running the Advanced Process Analysis System, the first window presented to the user is the 'Advanced Process Analysis Desk'. This is shown in Figure 9.

By default, the Advanced Process Analysis System opens a new model named 'untitled.ioo' in the program directory. The complete filename for this new model is shown in the bottom left corner of the window. The bottom right corner shows the date and the time the program was started. The file menu provides various options such as opening a new or an existing model. This is shown in Figure 10. The 'Recent Models' item in the file menu maintains a list of last four recently used models for easy access.

The Advanced Process Analysis Desk has five buttons leading to the five component programs, which were described in earlier sections. All of these can also be called using the process menu at the top. This is shown in Figure 11.

When a new model is opened, only the 'Flowsheet Simulation' button is available. This is because the development of the process model using Flowsim is the first step in the implementation of the Advanced Process Analysis System. Until the flowsheet simulation part is completed, buttons for the other four programs remain dimmed and unavailable.

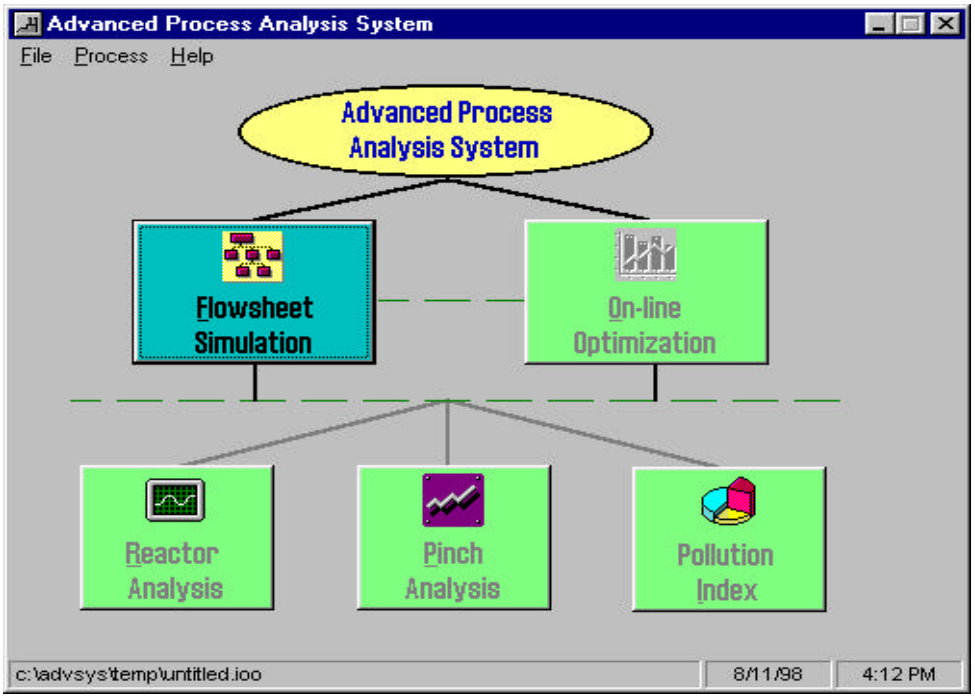


Figure 9 Advanced Process Analysis Desk

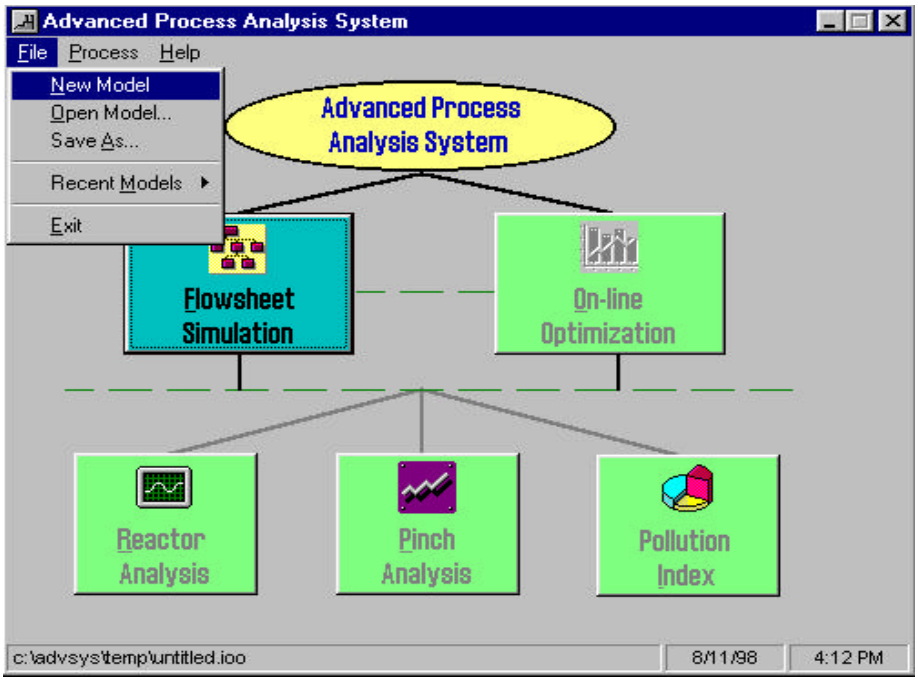


Figure 10 The File Menu of the Advanced Process Analysis Desk

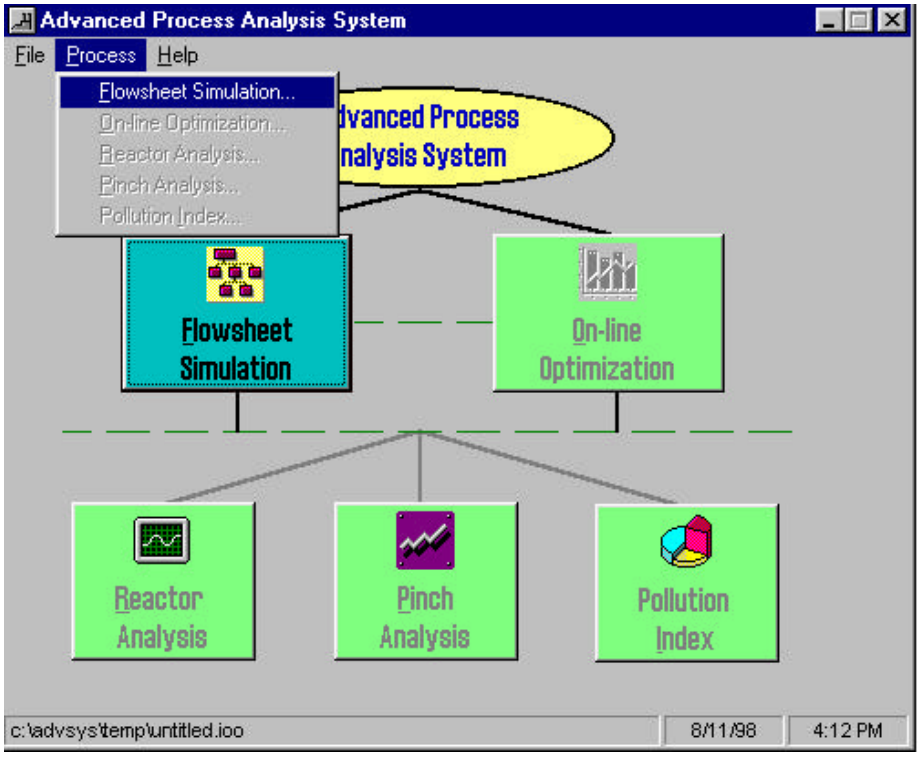


Figure 11 The Process Menu of the Advanced Process Analysis Desk

To implement the Advanced Process Analysis System for the Aniline process described in earlier section, the first step is to develop the process model using the Flowsim program. The 'Flowsheet Simulation' button should be now clicked to open the Flowsim program.

V. USING FLOWSIM

Upon clicking the 'Flowsheet Simulation' button in Figure 11, the FlowSim window is displayed with the 'General Information' box. In the space for model name, let us enter 'Aniline'. In the process description box, let us enter 'Ammonolysis of phenol simulation'. The 'General Information' box with this information is shown in Figure 12.

By clicking the 'OK' button, the main screen of 'FlowSim' is displayed. This is the screen where the user draws the flowsheet diagram. The 'Model' menu shown in Figure 13 provides the various commands used to draw the flowsheet diagram. The menu commands are divided into two groups. The first group has commands for drawing the flowsheet diagram whereas the second group has commands for entering various kinds of process information.

The 'Add Unit' command should be used to draw a process unit. The 'Add Stream' command should be used to draw a process stream between two process units. The program requires that every stream be drawn between two units. However, the input and output streams of a process only have one unit associated with them. To solve this problem, the FlowSim program provides an additional type of unit called 'Environment I/O'. This can be drawn using the command 'Add Environment I/O' in Figure 13. The 'Lock' option makes the diagram read-only and does not allow any changes. The diagram can be unlocked by clicking on the command again.

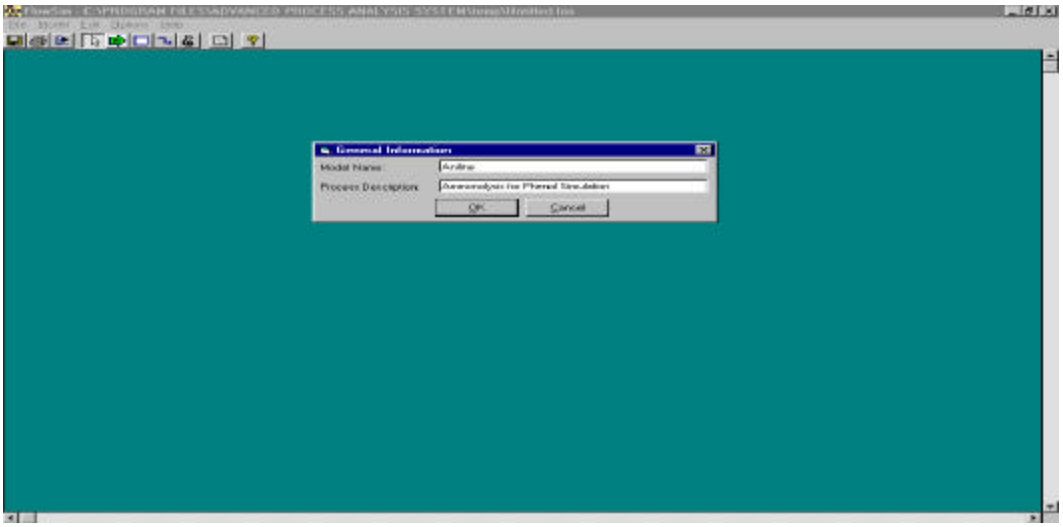


Figure 12 General Information Box

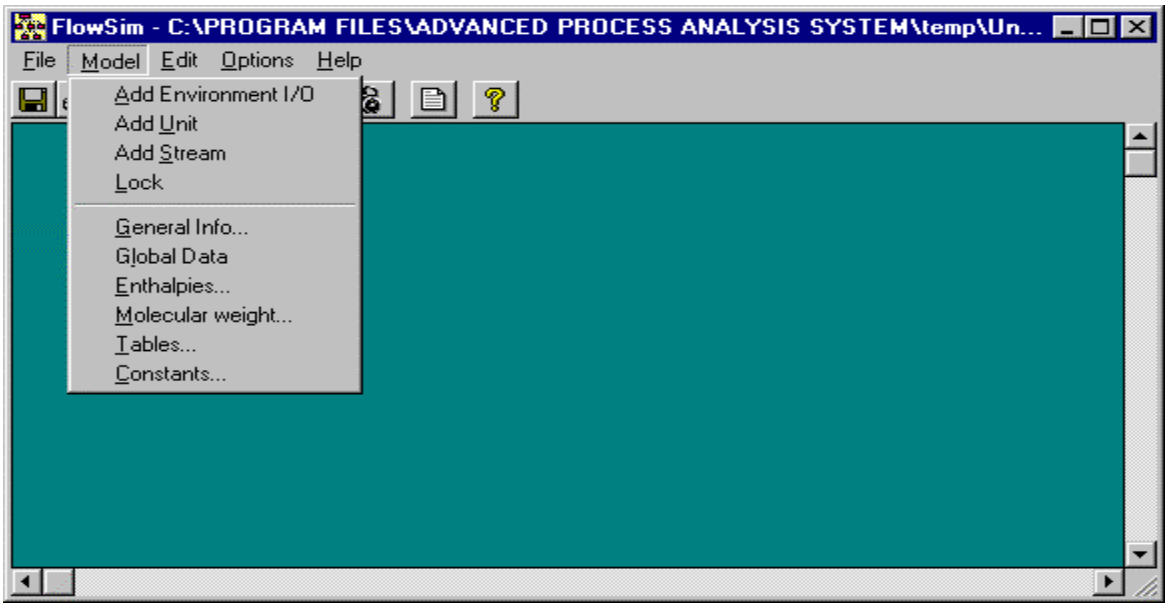


Figure 13 The Model Menu

Now, let us use these commands to draw the flowsheet diagram for the aniline process. Although FlowSim allows the units and streams to be drawn in any order, it is recommended that while drawing a process model, one should start with the feed and then add units and streams in order. Let us draw the mixer, which is the unit with the two feed streams and the two recycle streams as inputs. Select the 'Add Unit' command from the 'Model' menu. The mouse cursor changes to a hand. The cursor can now be dragged to draw a rectangle. Once, the mouse button is released, a small input window appears on the screen as shown in Figure 14. For every process unit that is drawn in FlowSim, the user is required to enter a unique Unit ID and description. let us enter 'MIX-102' as the unit ID and 'Feed and recycle mixer' as the description.

Now, let us draw the cross heat exchanger in the flowsheet diagram. Let us enter the Unit ID 'E-100' and description 'Cross heat exchanger'. With these two units, the screen looks like in Figure 15.

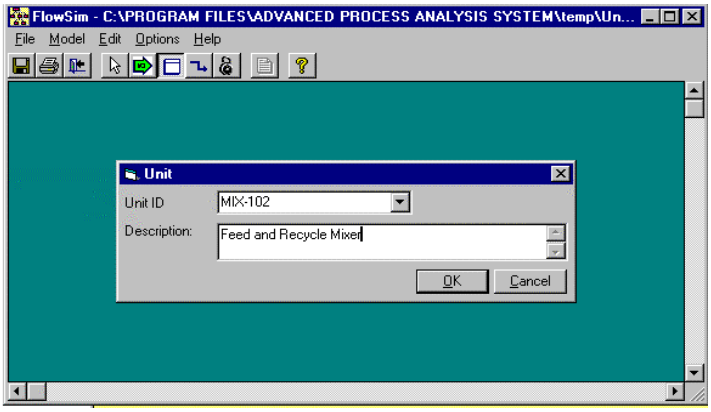


Figure 14 The Unit Window

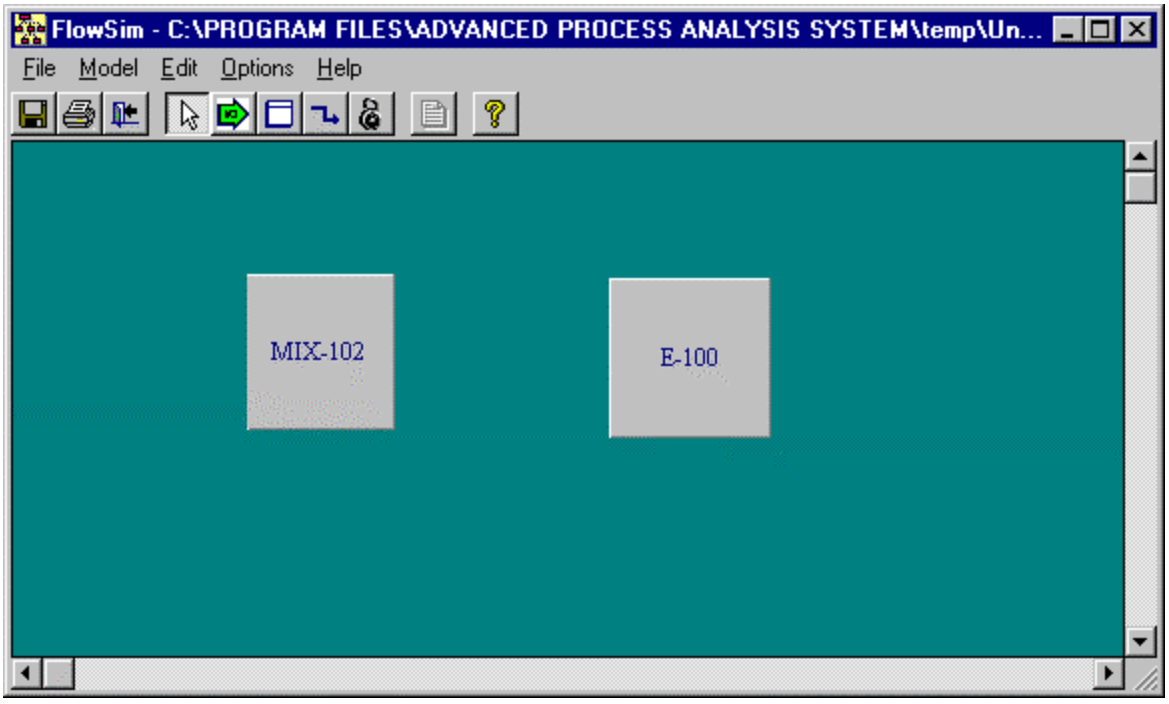


Figure 15: Flowsheet Screen with two Units.

Now, let us add the stream that leaves the mixer and enters the cross heat exchanger. To do this, select the 'Add stream' command from the 'Model' menu. The cursor changes to a small circle. Position the cursor on the MIX-102 unit and drag the cursor to the E-100 unit. The program now displays a small box shown in Figure 16. Let us enter the stream ID 's07' and the description 'Mixed stream'. With units MIX-102 and E-100 and stream s07, the FlowSim screen looks as shown in Figure 17. In this way, the entire process flow diagram for the sulfuric acid process can be drawn using the Model menu commands. After drawing the complete diagram, the FlowSim Screen Looks like as shown in Figure 18.

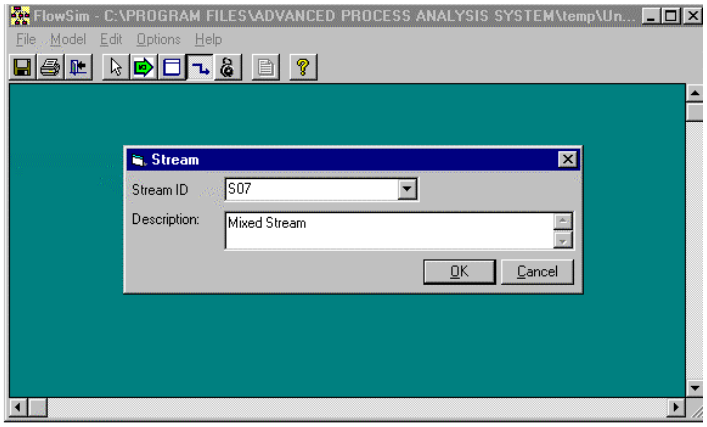


Figure 16. The Stream Window

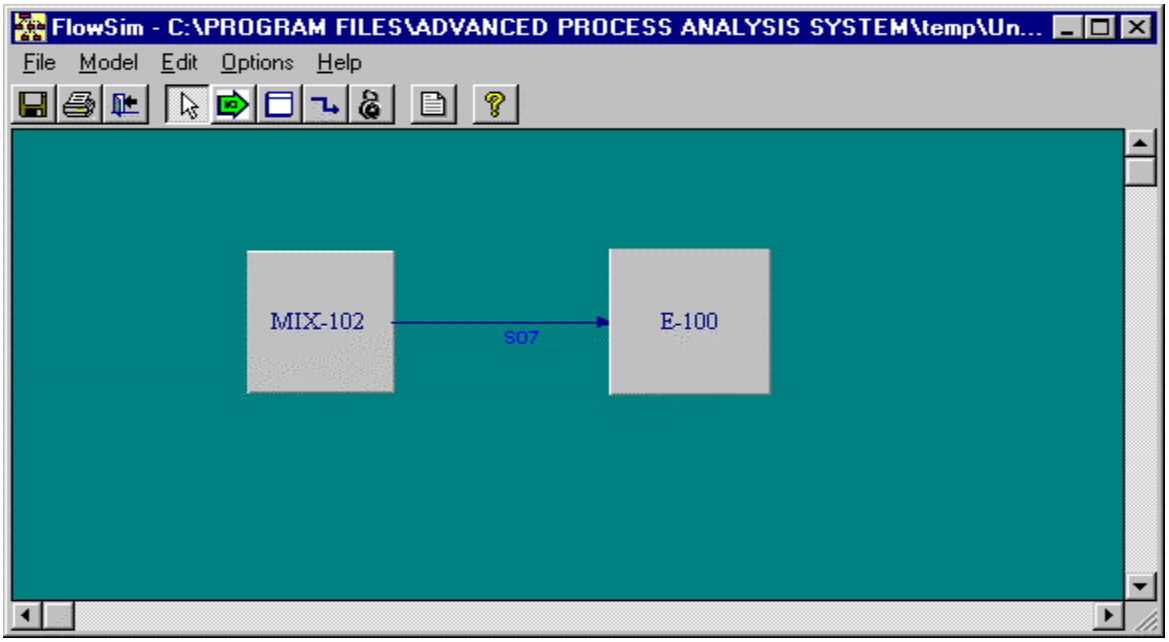


Figure 17. FlowSim Screen with two Units and a Stream

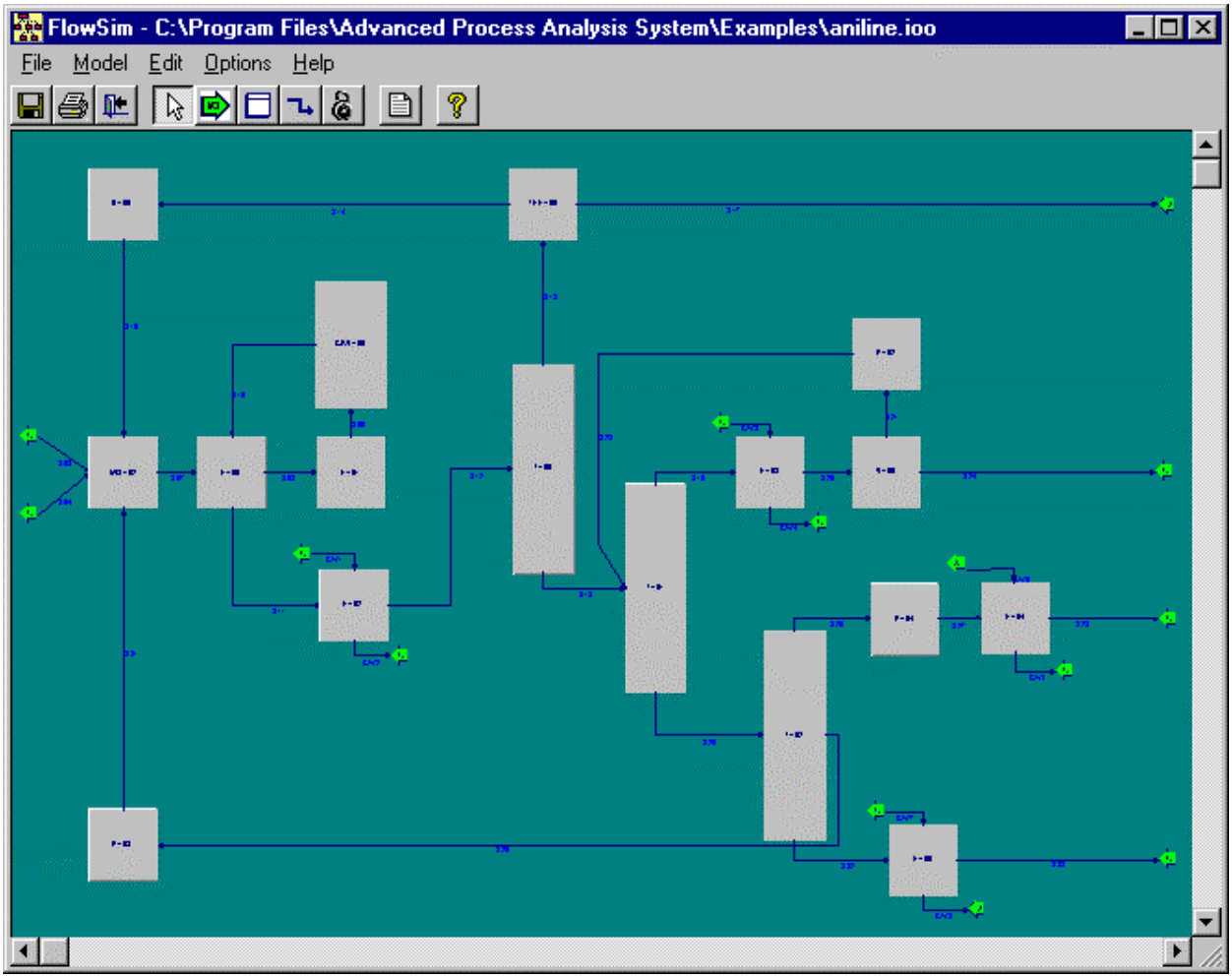


Figure 18 The Flowsim Screen with the Complete Process Diagram for Aniline Process Model

The 'Edit' menu at the top of the FlowSim screen provides various options for editing the diagram. It is shown in Figure 19. To use the Edit commands, a unit in the flowsheet diagram has to be selected first by clicking on it. The cut, copy and paste commands can be used for both units as well as streams. The 'Delete' command can be used to permanently remove a unit or a stream from the diagram. The 'Rename' command can be used to change the unit ID for a unit or to change the stream ID for a stream. The 'Properties' command can be used to change the appearance of a unit or a stream.

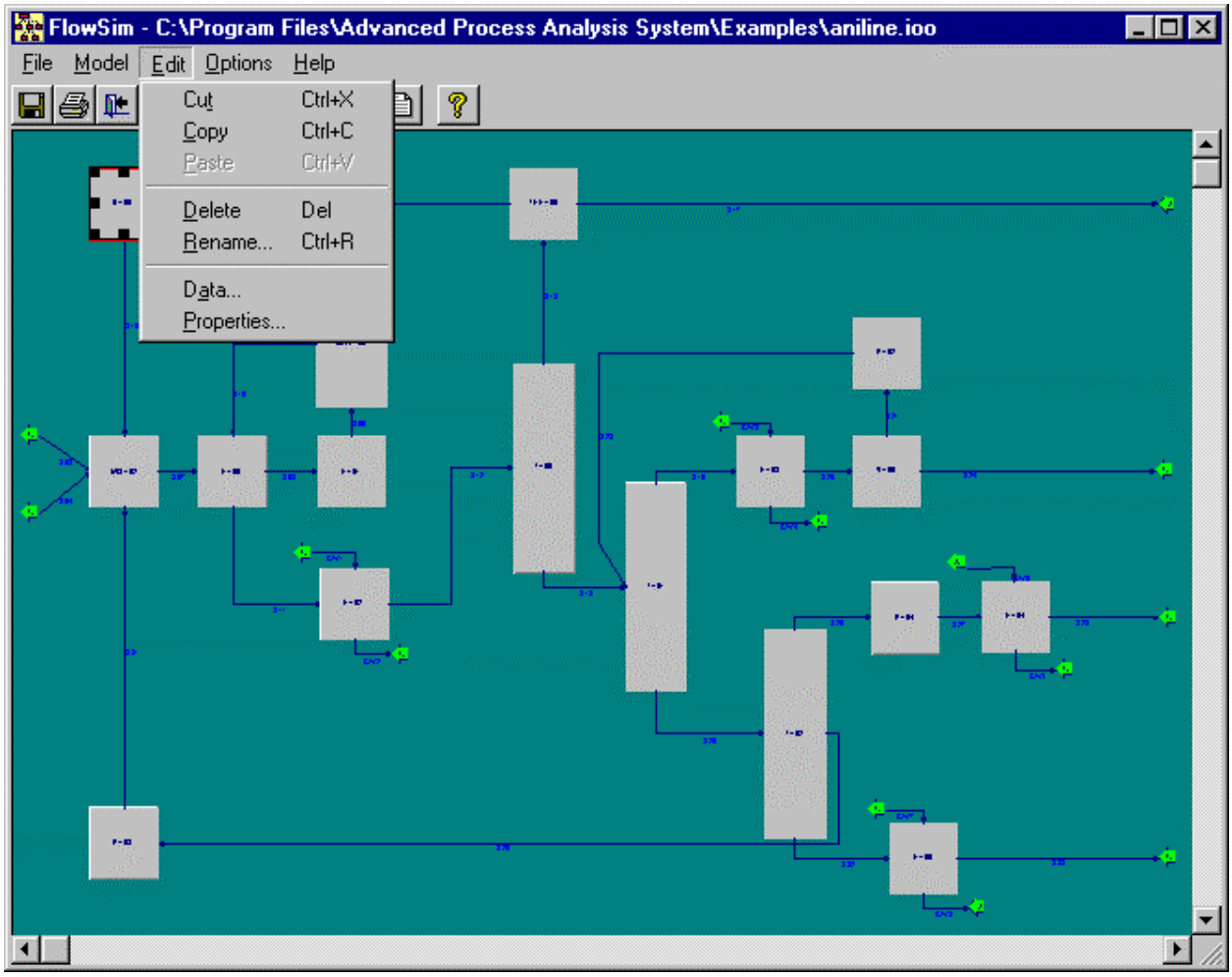


Figure 19 The Edit Menu

The 'Options' menu in the FlowSim screen is shown in Figure 20. The zoom option can be used to change the magnification by zooming in and out. The 'zoom to fit' option will automatically select the appropriate magnification so that the diagram occupies the entire screen. The 'Grid Lines' command can be used to display grid lines on the FlowSim screen, to change the spacing between the grid lines and to change the grid line and background colors. The 'Object settings' command is useful to change the appearance of all the units and streams in the FlowSim screen. The object settings window is shown in Figure 21. To change settings for all the streams, click on the streams tab. To change settings for all the environment I/O units, click on the 'Environment I/O' tab. If you want the changes to remain effective even after you close the application, you must select 'Save the palette for future uses' box.

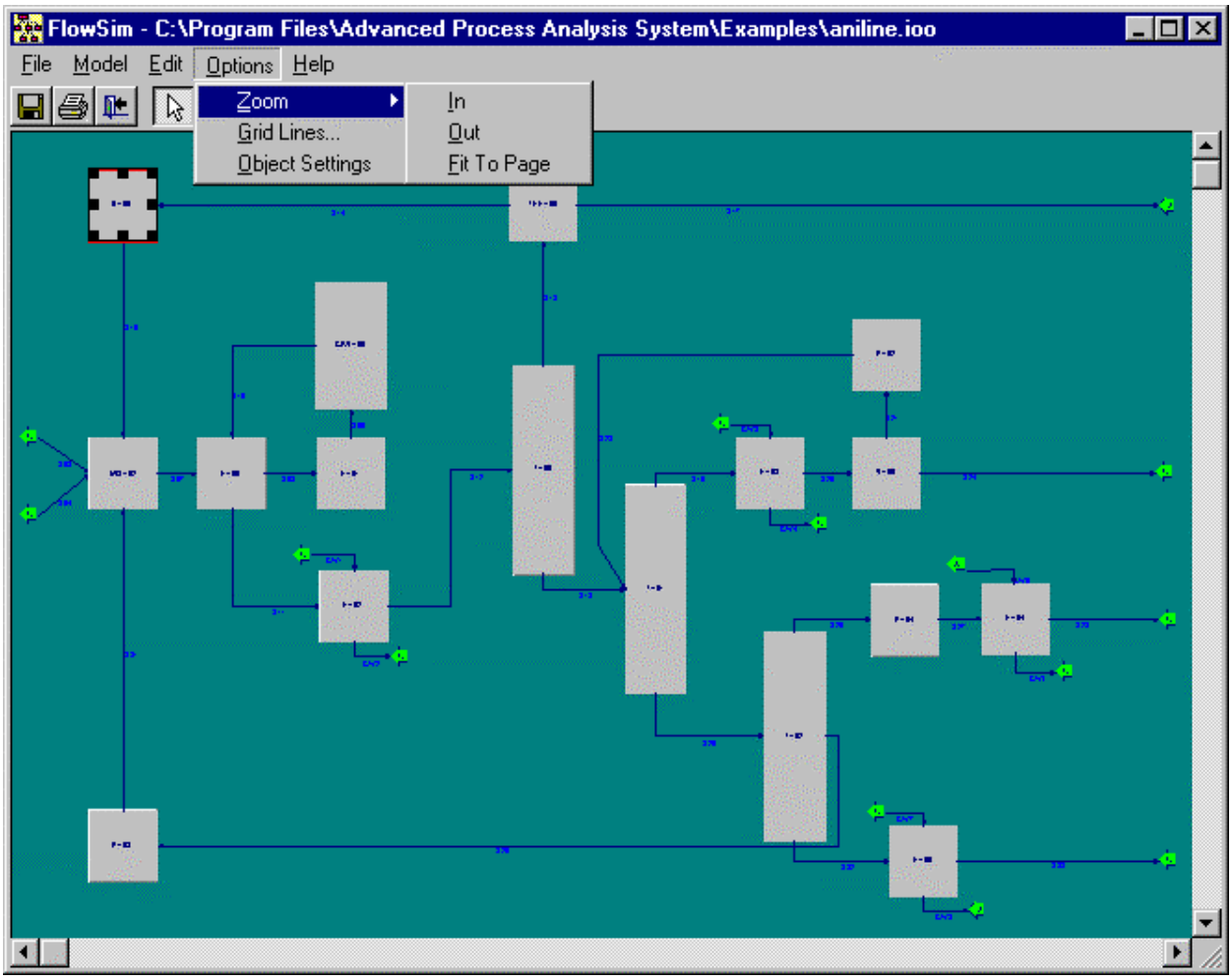


Figure 20 The Options Menu

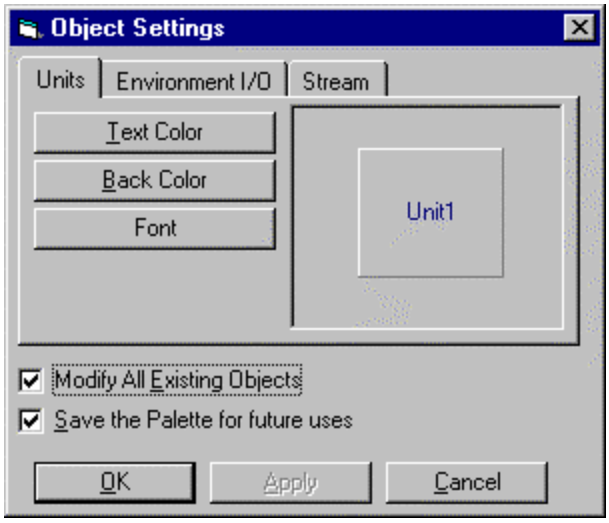


Figure 21 Object Settings Window

Once you have drawn a stream, the data associated with the stream can be entered by clicking on the data option in the edit menu or by double clicking on the stream. Let us enter the data associated with the stream s07. When you double click on this stream, a data form is opened. This is shown in Figure 22.

To enter the measured variables associated with the stream, the 'add' button should be clicked. When the 'add' button is clicked, the caption of the 'Refresh' button changes to 'Cancel'. Then the information about the variable such as the name of the variable, the plant data, the standard deviation of the plant data should be entered. The description, initial point, scaling factor, lower and upper bounds and the unit of the variable are optional.

The changes can be recorded to the model by clicking on the 'Update' button or can be cancelled by clicking on the 'Cancel' button. When the update button is clicked, the caption of the cancel button reverts back to 'Refresh'. The Stream Data Window with the information appears as shown in Figure 22. In this way, all the other measured variables associated with the stream 's07' can be entered

To enter the unmeasured variables associated with the stream, click on the 'Unmeasured Vars' tab. As explained above for the measured variables, click on the add button in the stream data window. Enter the name, initial point of the unmeasured variable. The bounds, scaling factor, description and unit of the variable are optional. The Stream Data window with the unmeasured variable data is shown in Figure 23.

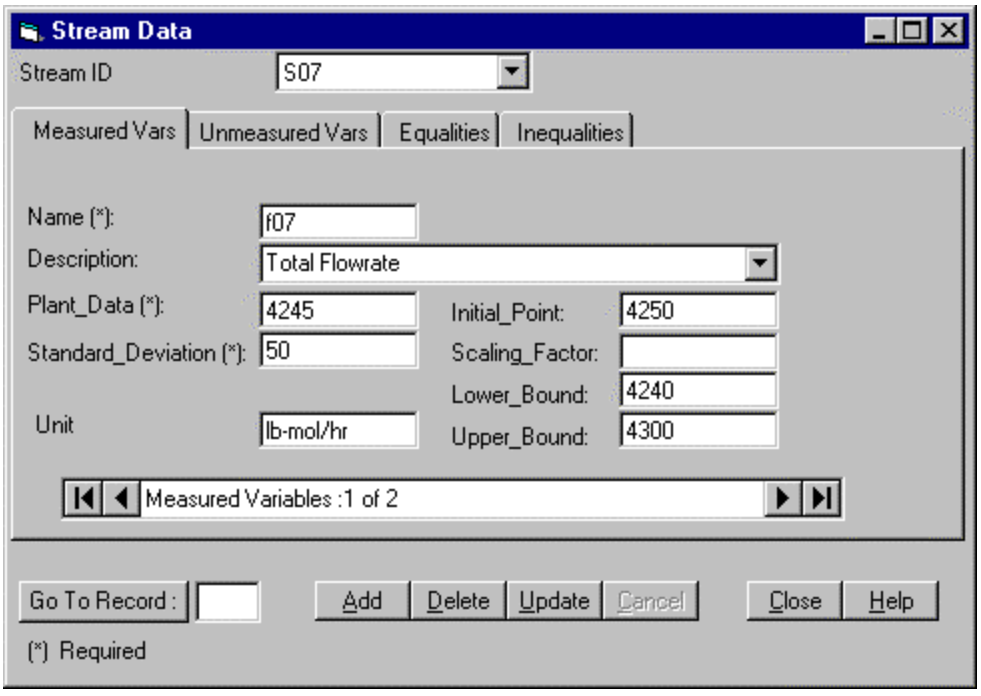


Figure 22 Stream Data Window

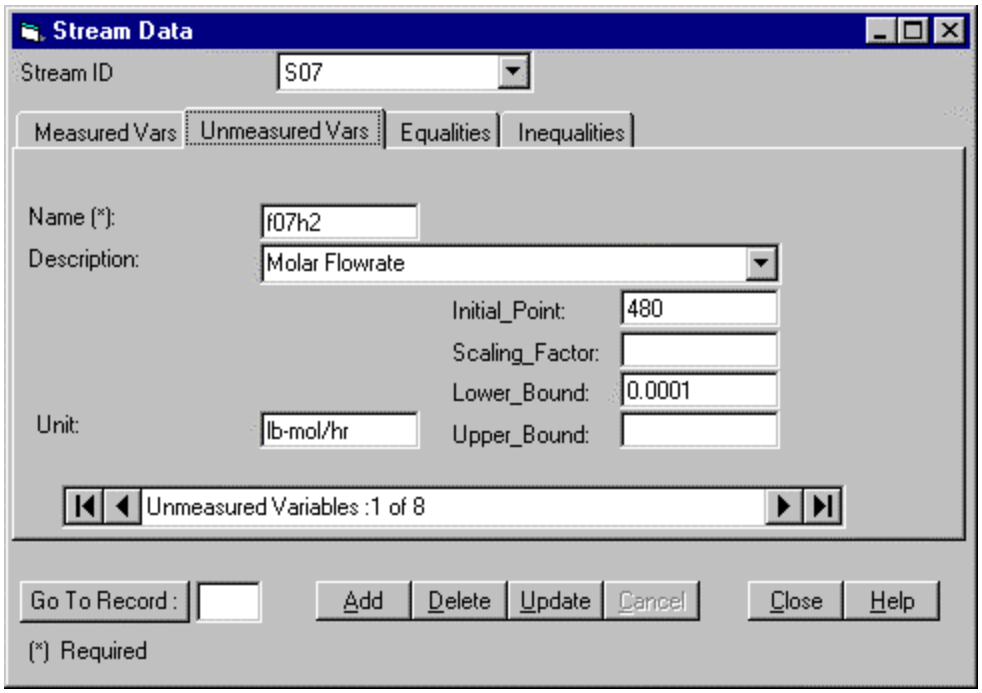


Figure 23 Unmeasured Variables Tab in the Stream Data Window

To move to a particular variable, enter the record number in the box adjacent to 'Go to Record' button. Then press 'enter' or click on the 'Go to Record' button to move to that variable. To delete a variable, first move to that variable and then click 'Delete'. To return to the main screen, click on the 'close' button.

To enter the data associated with a unit, double click on the unit. When you double click on the unit, a data form similar to the one shown in Figure 22 is opened. The measured variables, unmeasured variables are entered in the same way as for the streams.

Let us proceed to enter the equality constraints for the Cross heat Exchanger unit. Click on the Equalities tab in the Unit Data window to enter the equality constraints.

Let us enter the energy balance equation for the cross heat exchanger. This equation is given in Section XII. Click on the add button on the Unit Data window. Enter the equation in the box provided and click 'Update'. Note the use of '=e=' in place of '=' as required by the GAMS programming language. The screen now looks as shown in Figure 24-a

Let us enter the heat transfer equation for the cross heat exchanger. This equation is also given in Section XII. The Equality constraints tab in the Unit Data window for the cross heat exchanger with this equation is shown in Figure 24-b.

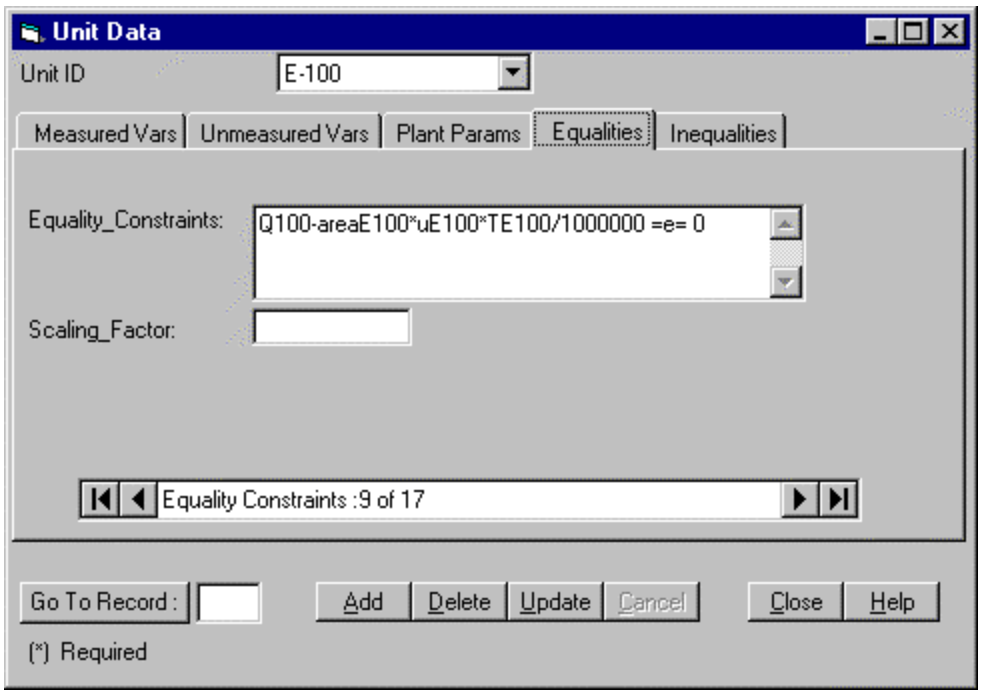


Figure 24.a: Equality Constraints Tab in the Unit Data Window

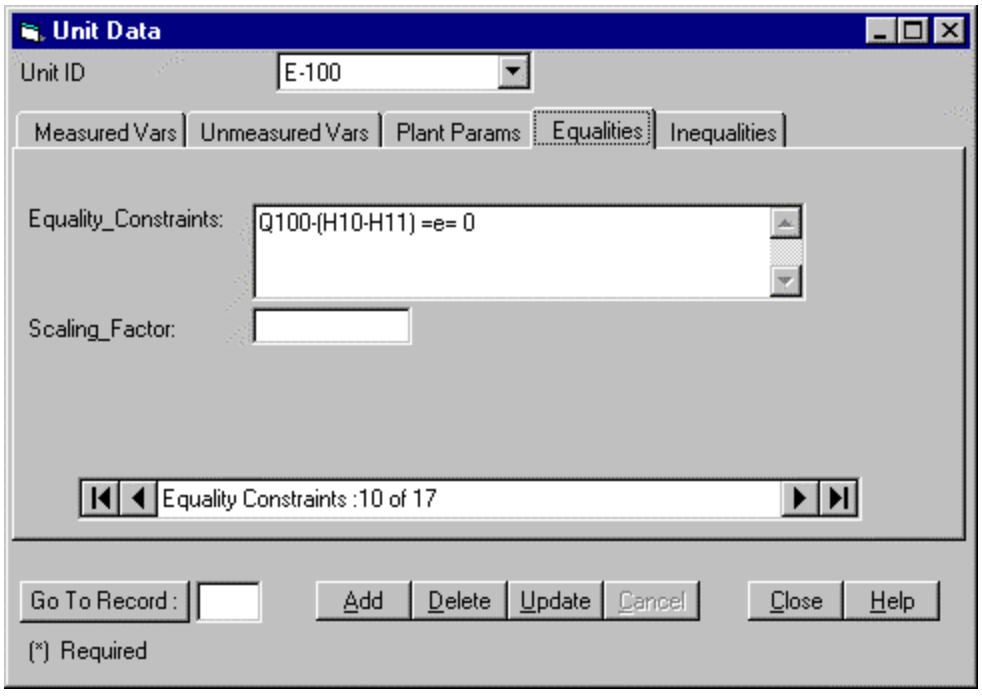


Figure 24.b: Equality Constraints Tab in the Unit Data Window

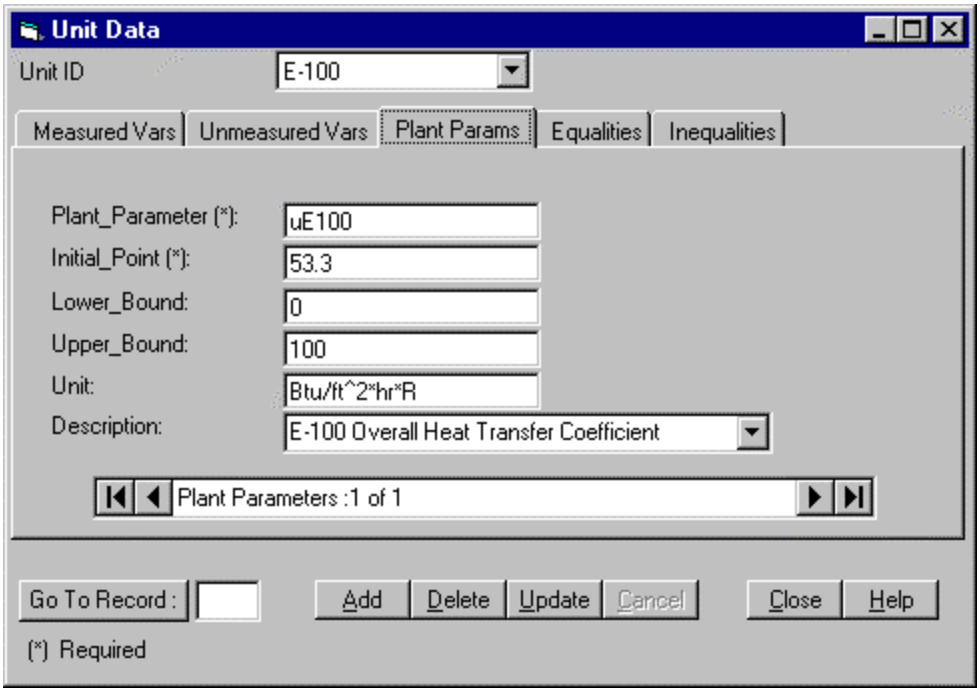


Figure 25 Plant Parameters tab in the Unit Data window

The Unit Data window has an extra tab for entering the parameters in the model, which are associated with that particular unit. Let us enter the parameter for the cross heat exchanger. Double click on the unit to open the Unit Data window. In the Unit Data window, click on the 'Plant Params' tab. Then, click on the 'Add' button. The parameter name and the initial point are required. Enter 'uE100' as the parameter name. This is the overall heat transfer coefficient of the exchanger. The bounds, description and the unit of the parameter are optional. The Unit Data window with the parameter information is shown in Figure 25.

A. Global Data

If there are variables, parameters and equations that do not belong to either a unit or a stream, then they can be entered in the Global Data window. This includes the economic model and the equations to evaluate emissions and energy use. To enter this global data, double click on the background of the flowsheet diagram or click on the 'Global Data' option in the Model menu.

The Global Data window in Figure 26-a shows the equality constraints in the Global Data section for the aniline process model . There are no equality constraints in the Global Data section for an aniline process so the window in Figure 26.a shows empty in the equality constraint section .

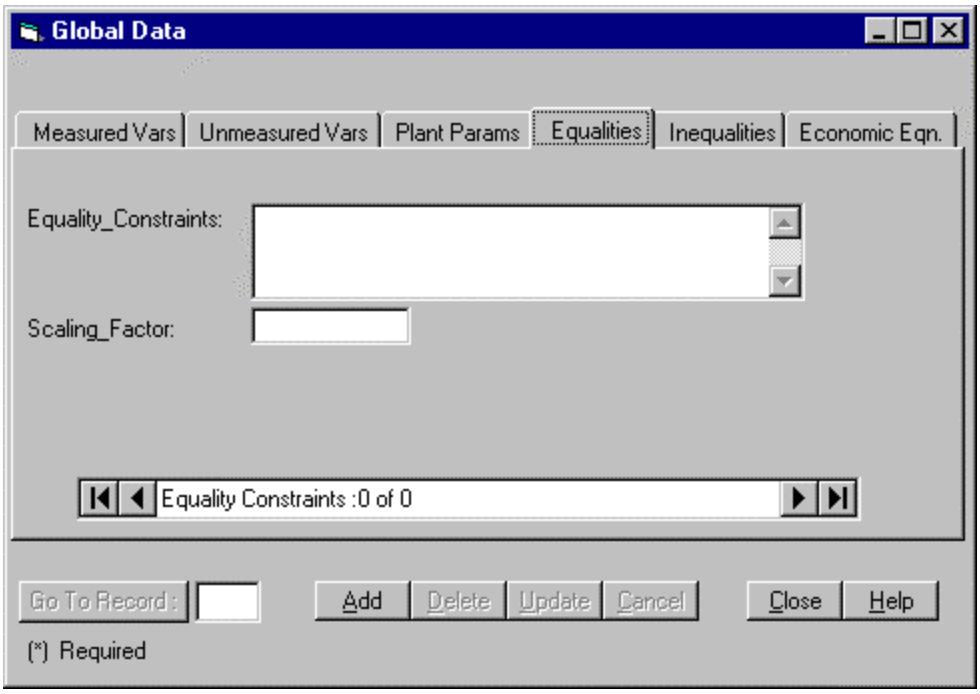


Figure 26.a Equalities Tab in the Global Data Window

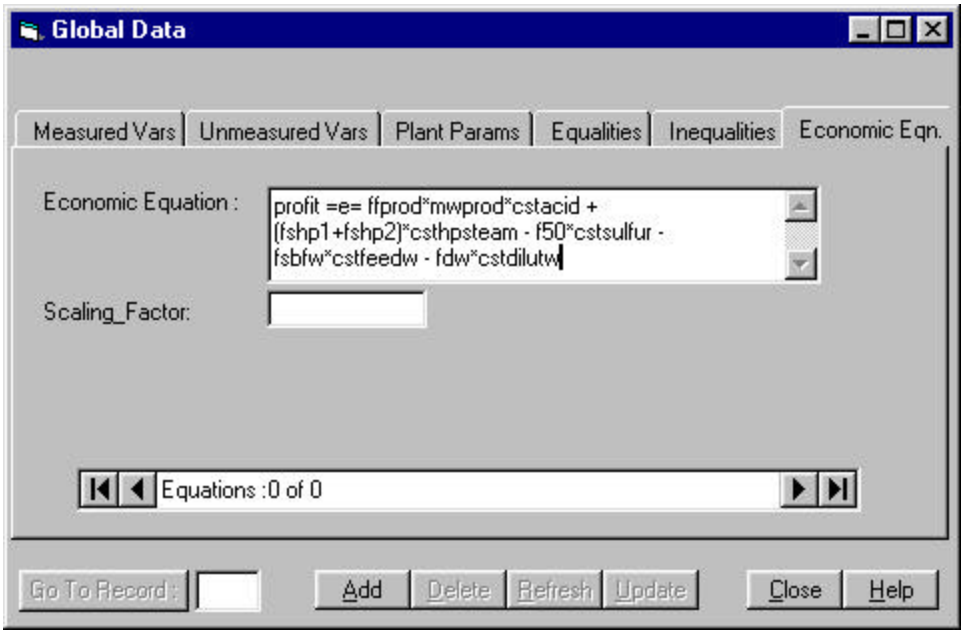


Figure 26.b The Economic Equations Tab of Global Data

The last tab in the Global Data window is for the Economic Equations. These are equations, which can be used as the economic model and the left-hand side of one of these equations is specified in on-line optimization as discussed in Section VI. For the aniline process, let us enter the equation that defines the profit function for the whole process. Click on the 'Add' button and enter the equation shown in Figure 26-b. The variable 'profit' will be used later to specify the objective function for economic optimization. As seen in Figure 26-b, the profit function is equal to the product stream flowrates (lb/hr) multiplied by their sales coefficients ($/lb) subtracted by the input stream flowrates (lb/hr) multiplied by their cost coefficients ($/lb).

B. Tables

If there are constant coefficients used in the constraints equations, they can be defined as a table. These constant coefficients are grouped in sets, and they can be defined using concise names to refer their values in the equations before an equation definition. Let us create a new table for the Contact model. Click on the 'Tables' option in the model menu to open the Tables window, which is shown in Figure 27. Then click on the 'Add New' button in the tables window to activate the window. As soon as 'Add New' button is clicked, the caption of the 'Add New' button changes to 'Save' and that of 'Delete' changes to 'Cancel'. Then the general information of a table - the name of the table, number of rows and number of column names - must be entered. The name of the table stands for the name of the coefficient group. The names of the rows and columns are the set names of the sub-components. After entering the table information, the 'Save' button should be clicked to save the changes.

To enter data in a table, click on the 'Edit' button. The Edit Table window is opened to enter names and numerical values for the constant coefficients. The edit table window for the table 'enth_gas' is shown in Figure 28. Clicking the 'Close' button will update the table and close the 'Edit table' window. An existing table can be edited or deleted by selecting the table and then clicking 'Edit' or 'Delete'

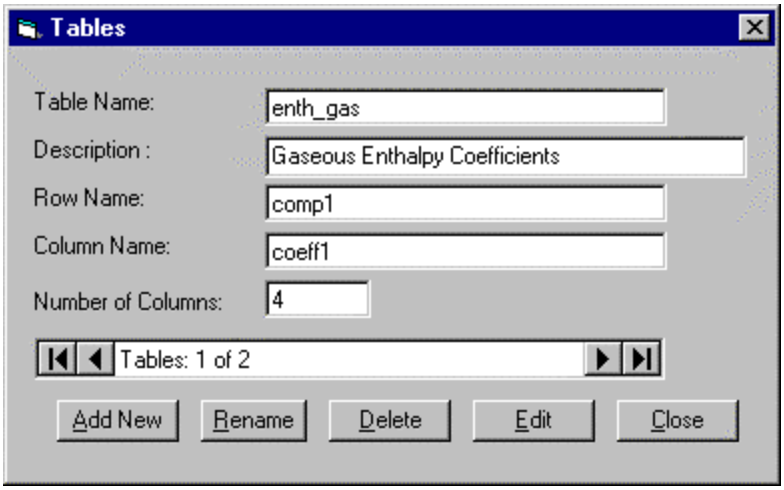


Figure 27 Table Window

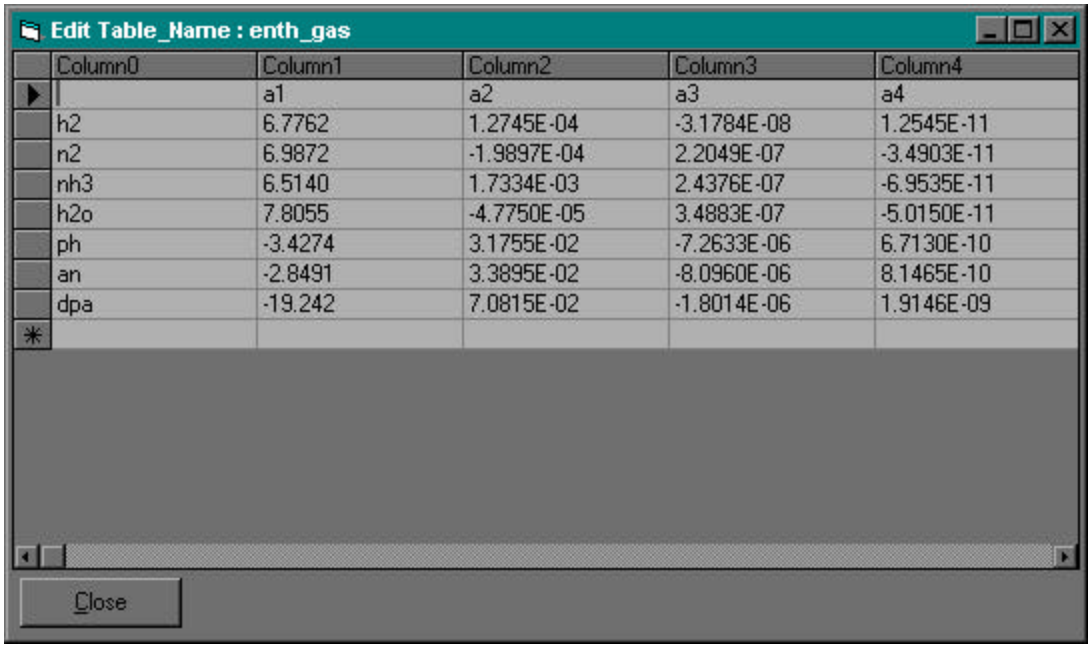


Figure 28 Edit Table Window

C. Enthalpies

The enthalpy of a stream usually is expressed as a polynomial function of temperature. This function appears repeatedly in the plant model with the same coefficients, which have different numerical values for each chemical component. An example is:

$$h_i = a_{0i} + a_{1i}T + a_{2i}T^2 + a_{3i}T^3 + a_{4i}T^4$$

where there are six coefficients, a_{0i} to a_{5i}, for component i.

An enthalpy window can be used to store enthalpy coefficients for a group of components. To create an enthalpy table, click on the ‘Enthalpies’ option in the model menu to open the Enthalpy window. Then click on the ‘'Add New' button in the Enthalpy window. As soon as the user clicks on ‘Add New’ button, an input window prompts the user to enter the name of the enthalpy table, a description of the enthalpy table, the row name and the column name. An enthalpy table with the given name is created. An enthalpy table can be deleted by clicking on the ‘Remove’ button. The enthalpy window is shown in Figure 29.

The enthalpy coefficients from the Enthalpy table can be used in the enthalpy equations written in the FlowSim part of the program. However, the Enthalpy table does not write the equations for the user. The calculations in the Pinch Analysis and Reactor Analysis parts of the Advanced Process Analysis program also utilize the coefficients from the Enthalpy table. It is recommended that separate tables be used for different phases of the same component.

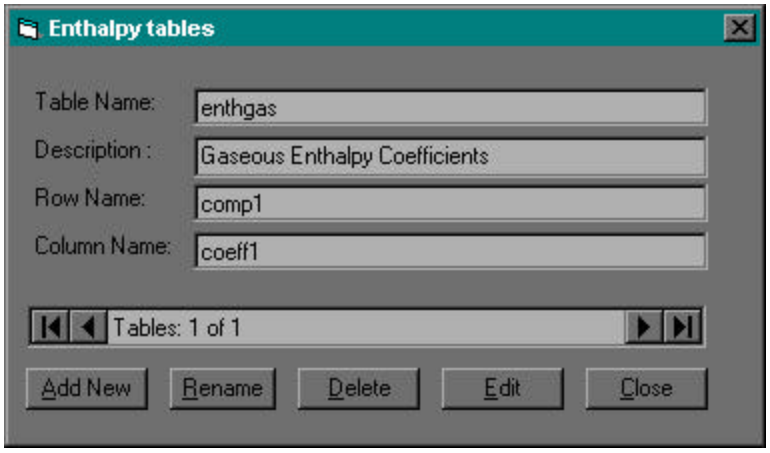
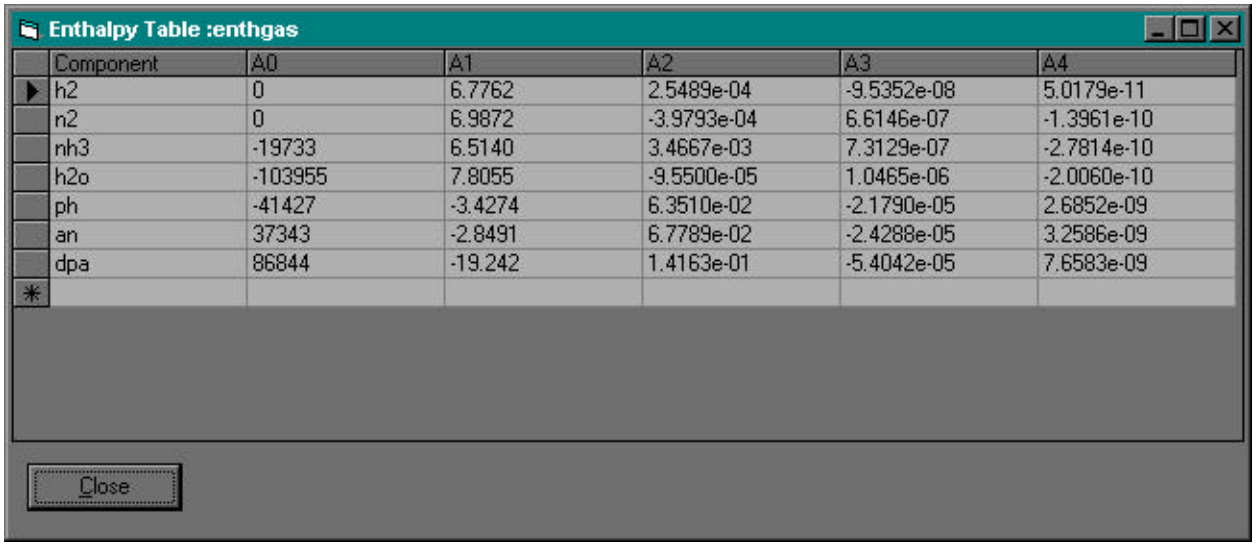


Figure 29: Enthalpy Window



Component	A0	A1	A2	A3	A4
h2	0	6.7762	2.5489e-04	-9.5352e-08	5.0179e-11
n2	0	6.9872	-3.9793e-04	6.6146e-07	-1.3961e-10
nh3	-19733	6.5140	3.4667e-03	7.3129e-07	-2.7814e-10
h2o	-103955	7.8055	-9.5500e-05	1.0465e-06	-2.0060e-10
ph	-41427	-3.4274	6.3510e-02	-2.1790e-05	2.6852e-09
an	37343	-2.8491	6.7789e-02	-2.4288e-05	3.2586e-09
dpa	86844	-19.242	1.4163e-01	-5.4042e-05	7.6583e-09

Figure 30. Edit Enthalpy Table Window

Let us create a new enthalpy table for the Aniline model. Click on the 'Enthalpies' option in the model menu to open the Enthalpy Tables window, which is shown in Figure 31. Then click on the 'Add New' button in the Enthalpy Tables window to activate the window. As soon as 'Add New' button is clicked, the caption of the 'Add New' button changes to 'Save' and that of 'Delete' changes to 'Cancel'. Then the general information of a table - the name of the enthalpy table, the description of the enthalpy table, the row name and the column name - must be entered. After entering the table information, the 'Save' button should be clicked to save the changes.

To enter data in an enthalpy table, click on the 'Edit' button. The Edit Table window is opened to enter names and numerical values for the constant coefficients. The edit table window for the table 'enthgas' is shown in Figure 30. Clicking the 'Close' button will update the table and close the 'Edit table' window. An existing table can be edited or deleted by selecting the table and then clicking 'Edit' or 'Delete'.

D. Constant Properties

The Constant Property window is where a list of constants is stored. Clicking on the 'Constants' option in the model menu opens the Constant Property window as shown in Figure 31. To create a set of constant properties, click on the 'Add New' button in Constant Property window to activate the window. As soon as the 'Add New' button is clicked, the caption of the 'Add New' button changes to 'Save' and that of 'Delete' changes to 'Cancel'. Then the general information of a constant property - the name and an optional description - must be entered in the Constant Property window.

After entering the constant property information, the 'Save' button should be clicked to save the changes.

To enter the data in the constant property window, click on the 'Edit' button. The Edit Constant Property window is opened for entering the name of the constant, the corresponding numerical value and an optional description. The Edit Constant Property window is shown in Figure 32.

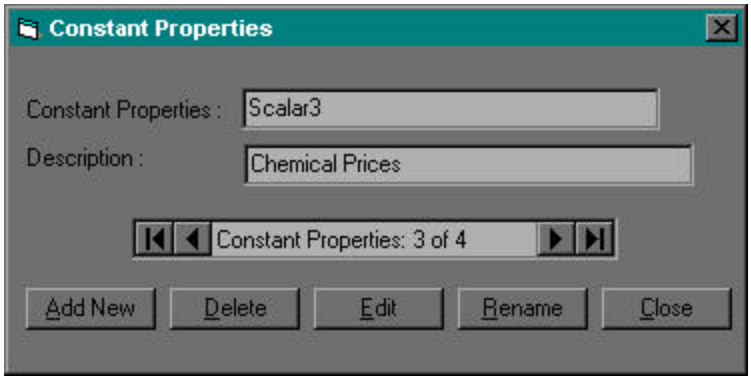


Figure 31 Constant Properties Window

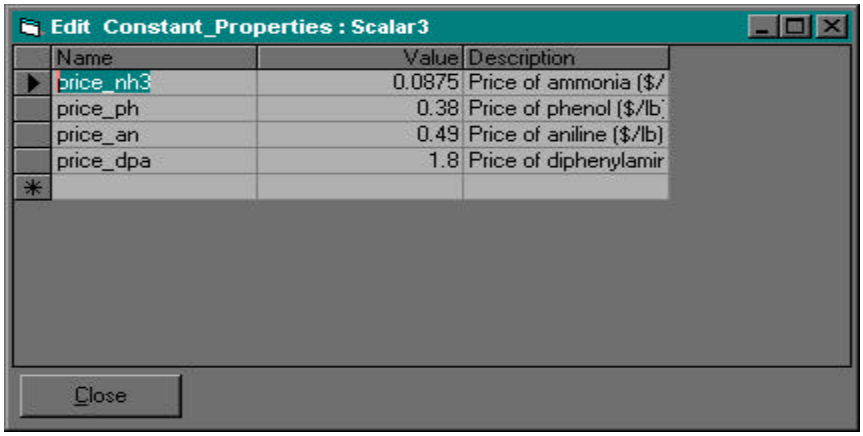


Figure 32 Edit Constant Property Window

E. Molecular Weight Table

The Molecular Weight Table window is where the molecular weights of the components are stored. Clicking on the 'Molecular Weight' option in the model menu opens the Molecular Weight Table window as shown in Figure 33.

The component names along with their Molecular Weight and Description are entered as shown in Figure 33. After clicking on the 'Close' button, this window is closed

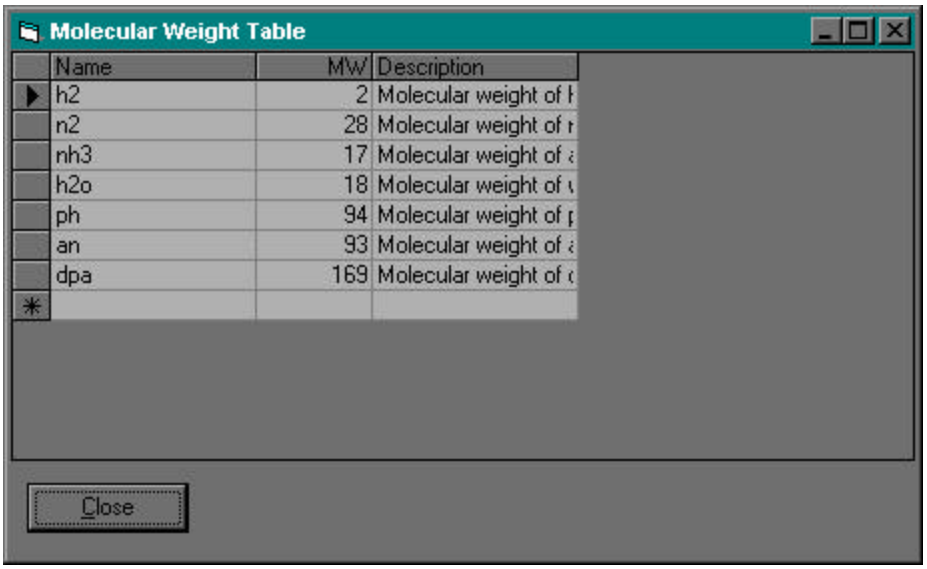


Figure 33 Molecular Weight Table

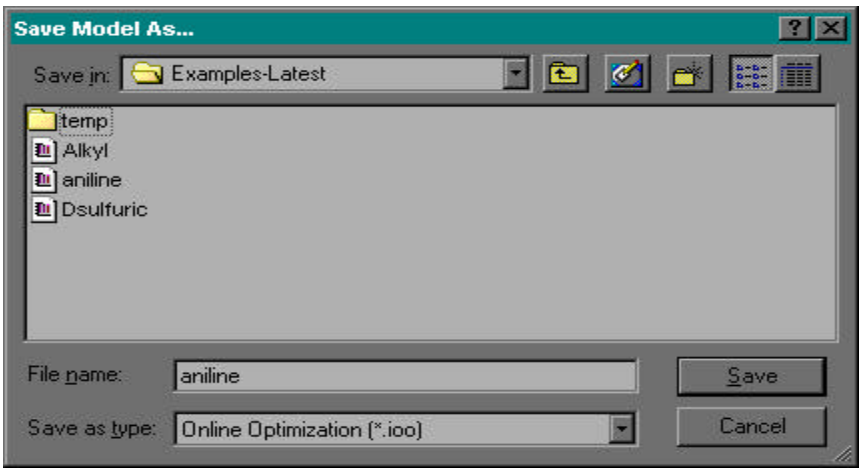


Figure 34. Save Model As Dialog Box

After entering all of the above information, the model is complete. Save the changes by clicking on the 'Save' option in the File menu. If you click 'Exit' without saving the model, a message is displayed asking whether you want to save the changes or not. The ‘Print’ option in the File menu when clicked, prints the flowsheet diagram. When the ‘Exit’ button is clicked, the FlowSim window is closed and the user is taken back to the Advanced Process Analysis Desk.

The development of the process model using FlowSim has been completed. The equations, parameters and constants have been stored in the database as shown in Figure 1. Save the model using the ‘Save As’ option in the File menu. A ‘Save Model As’ dialog box as shown in Figure 34 is opened. Save the model as ‘aniline.ioo’ in the ‘Examples’ subdirectory of the program folder.

The process model developed above needs to be validated to make sure that it is representing the actual process accurately and it does not have any mistakes. This can be done by using the model to carry out a simulation and then comparing the results with the design data for the process. If the design data is not available, an alternative solution is to use the combined gross error detection and data reconciliation step of on-line optimization to check the model validity. The plant operating data obtained from the distributed control system can be used for this purpose. The reconciled data obtained is compared with the plant data and if the values agree within the accuracy of the data, the model is an accurate description of the actual process. For the aniline process, this strategy is used to validate the model. The combined gross error detection and data reconciliation is the first step of on-line optimization and will be explained in the next section.

The next step of the Advanced Process Analysis System is on-line optimization. The ‘On-line Optimization’ button in Figure 9 should be now clicked to open the On-line Optimization program.

VI. USING ONLINE OPTIMIZATION PROGRAM

Upon clicking the 'On-line Optimization' button, the On-line Optimization main window is displayed with the Optimization Algorithm window as shown in Figure 35. This window includes the algorithms for Data Validation and Parameter Estimation, the Objective function for Economic Optimization, the Optimization direction and the Economic Model type. The default options are Tjoa-Biegler's method for data validation and Least Squares method for Parameter Estimation. In the Economic Optimization for the aniline process, the objective function is 'profit' as defined in Section V for the global economic equation (Figure 26-b). Let us choose the optimization direction to be 'Maximizing' and the Economic Model type to be 'Linear'.

When you click on the View menu in the Optimization Algorithm window, a pulldown menu is displayed as shown in Figure 36. The View menu includes commands for the Optimization Algorithm mode, the All Information mode and Flowsheet diagram. The 'Optimization Algorithm' mode displays the model description window. The 'All Information' mode contains the different windows combined together into one switchable window. The Flowsheet diagram option is used to view the flowsheet diagram, which is drawn using the flowsheet simulation program.

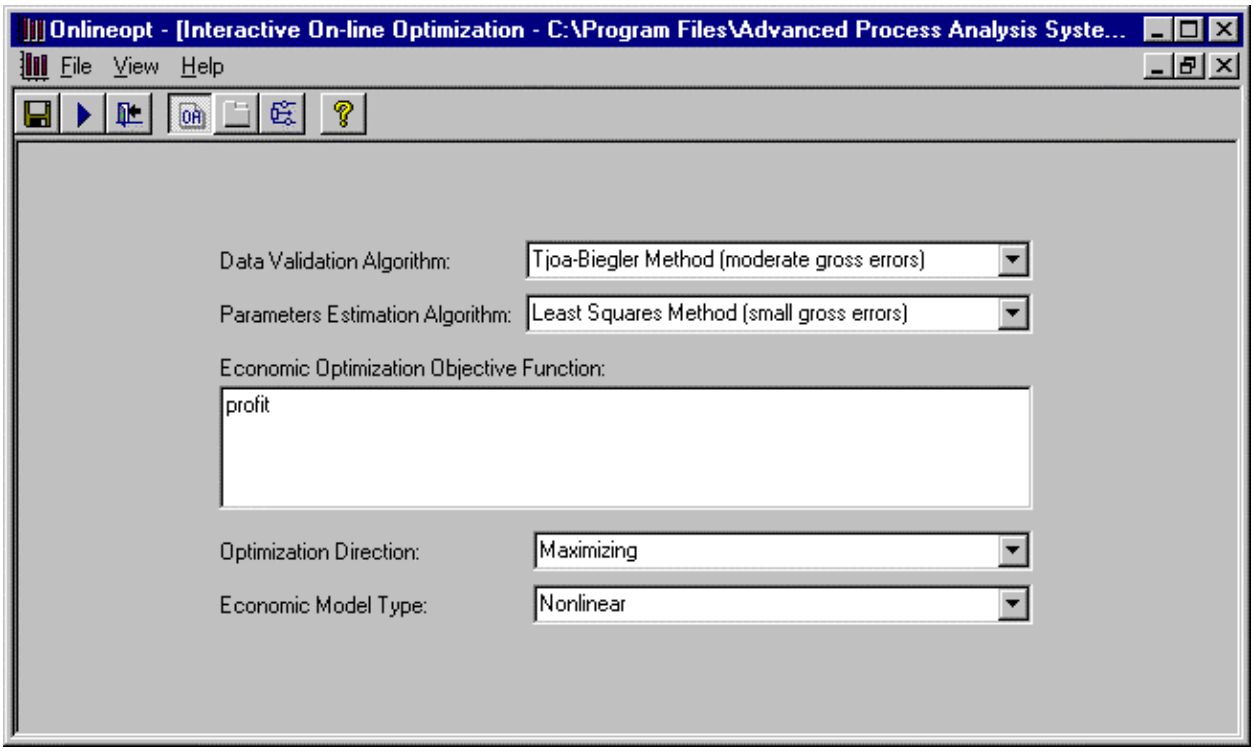


Figure 35:Online Optimization Algorithm Window

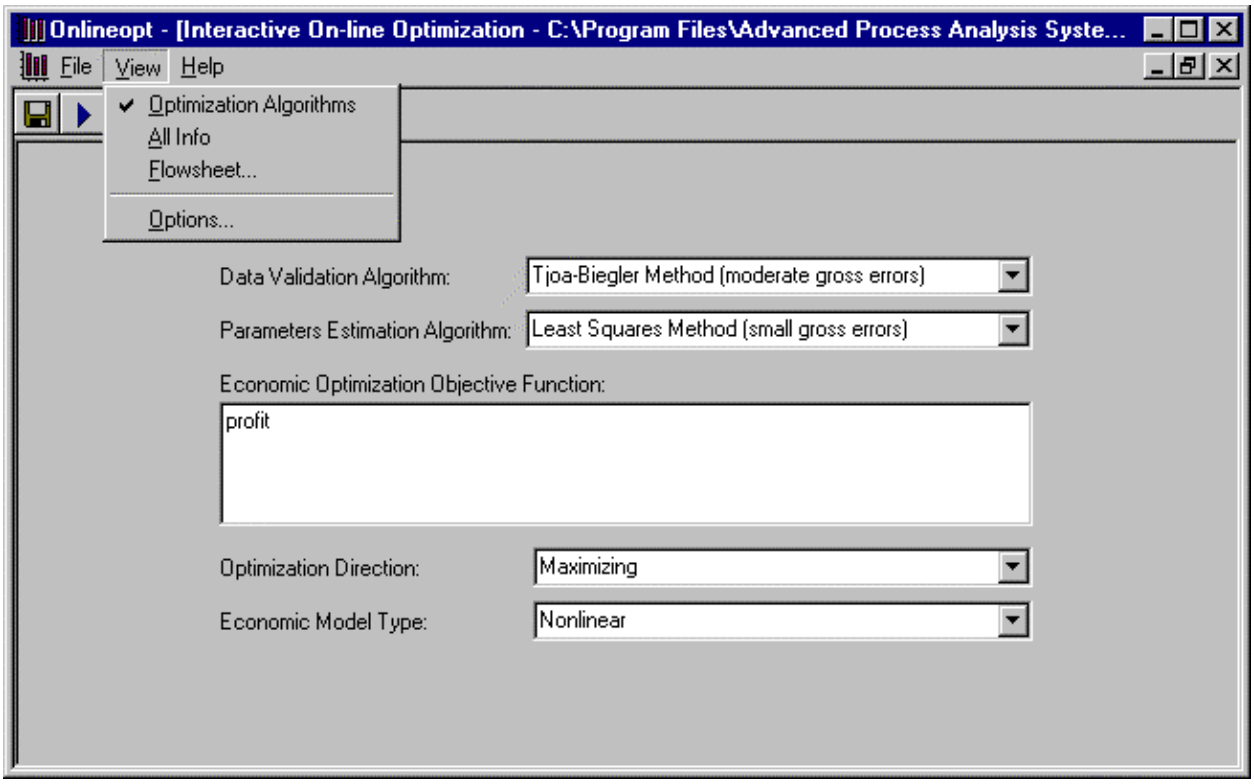


Figure 36 View Menu

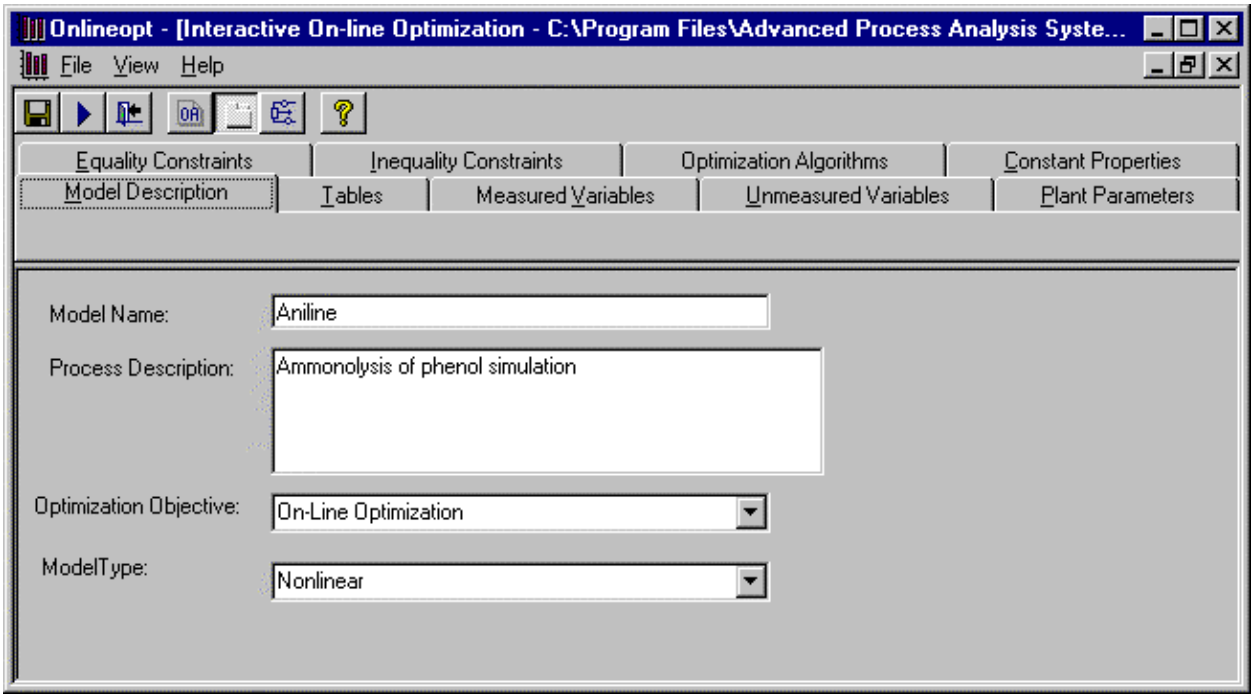


Figure 37 Model Description Window

To view the other windows used by the On-line Optimization program click on the ‘All Information’ option in the view menu which is shown in Figure 36. The Model Description window is shown in Figure 37.

For the Model Description window, the model name and the description were entered in the Flotsam program. This window includes the Optimization Objective and Model Type. The optimization objective can be selected from the drop-down list of 'Optimization Objective'. The five selections are 'On-line Optimization (All)', 'Data Validation', 'Parameter Estimation', 'Economic Optimization' and 'Parameter Estimation and Economic Optimization'. Let us choose the 'On-line Optimization (All)' option for the optimization objective. The model type of the plant model must be specified as either 'Linear' or 'Nonlinear' from the drop-down list. Let us choose 'Nonlinear' as the model type for the aniline model.

When the information for the Model Description window is completed, you can proceed to the next window by clicking on the tab to move to any other window. Let us proceed to the Tables window by clicking on the ‘Tables’ tab. The Tables window is shown in Figure 38; it contains information about the tables that were entered in the FlowSim program.

Let us proceed to the Measured Variables window by clicking the ‘Measured Variables’ tab. The Measured Variables window has a table with twelve columns which display the name, plant data, standard deviation, initial point, scaling factor, lower and upper bounds, stream number, process unitID, the unit and a short description of the measured variables. The Measured Variables window lists all the measured variables that are associated with all the units and streams in the process model and the global measured variables that were entered in the FlowSim program. The column ‘Process UnitID’ has the name of the process unit and the column ‘Stream Number’ has the name of the stream with which the variable is associated. The Measured Variables window is shown in Figure 39. In this window, information can only be viewed. All of the data entered in FlowSim can only be viewed using the screens of on-line optimization. To change the data, the user has to go back to the FlowSim program.

Then proceed to the Unmeasured Variables window by clicking on the ‘Unmeasured Variables’ tab. The Unmeasured Variables window has nine columns for displaying the name, initial point, scaling factor, lower and upper bounds, stream number, process unitID, unit and description of the unmeasured variables. The Unmeasured Variables window lists all the unmeasured variables, which were entered in the FlowSim program. The Unmeasured Variables window is shown in Figure 40.

Optimization programs need to have all the variables in the same numerical range, and it may be necessary to scale the variables by adjusting the scaling factors. To scale variables using the Scaling Option provided by the system, the scale factors must be entered in the FlowSim program and the icon ‘Include SCALING OPTION for variables’ at the bottom of Figure 39 for measured variables or Figure 40 for unmeasured variables should be checked. A description of scaling factors and their use is given in Section XI.

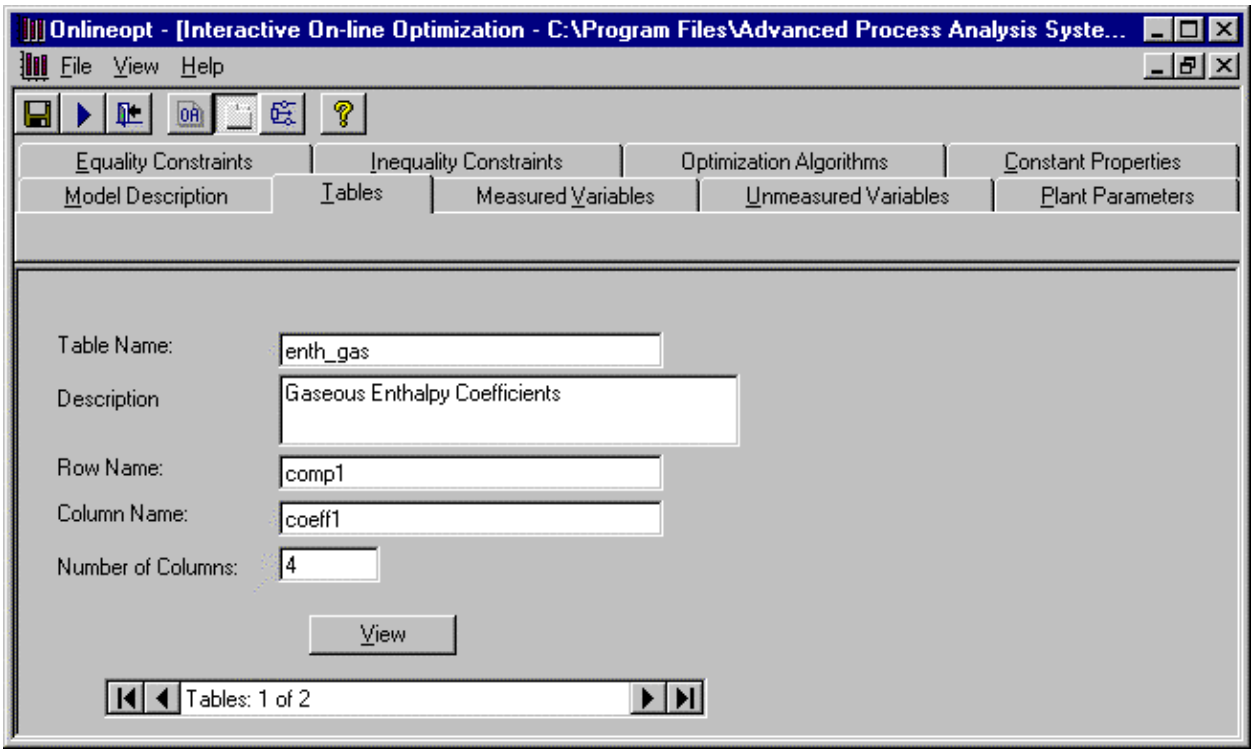
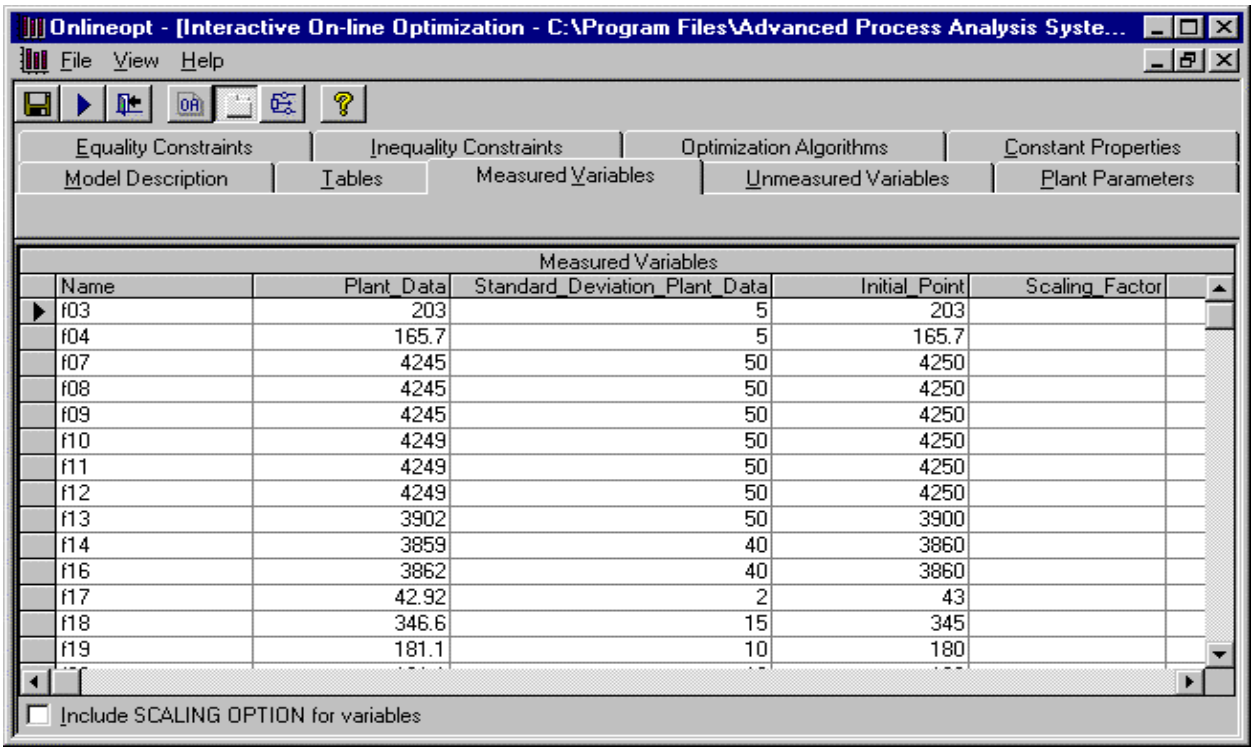


Figure 38: Tables Window



Name	Plant_Data	Standard_Deviation_Plant_Data	Initial_Point	Scaling_Factor
f03	203	5	203	
f04	165.7	5	165.7	
f07	4245	50	4250	
f08	4245	50	4250	
f09	4245	50	4250	
f10	4249	50	4250	
f11	4249	50	4250	
f12	4249	50	4250	
f13	3902	50	3900	
f14	3859	40	3860	
f16	3862	40	3860	
f17	42.92	2	43	
f18	346.6	15	345	
f19	181.1	10	180	

Figure 39: Measured Variables Window

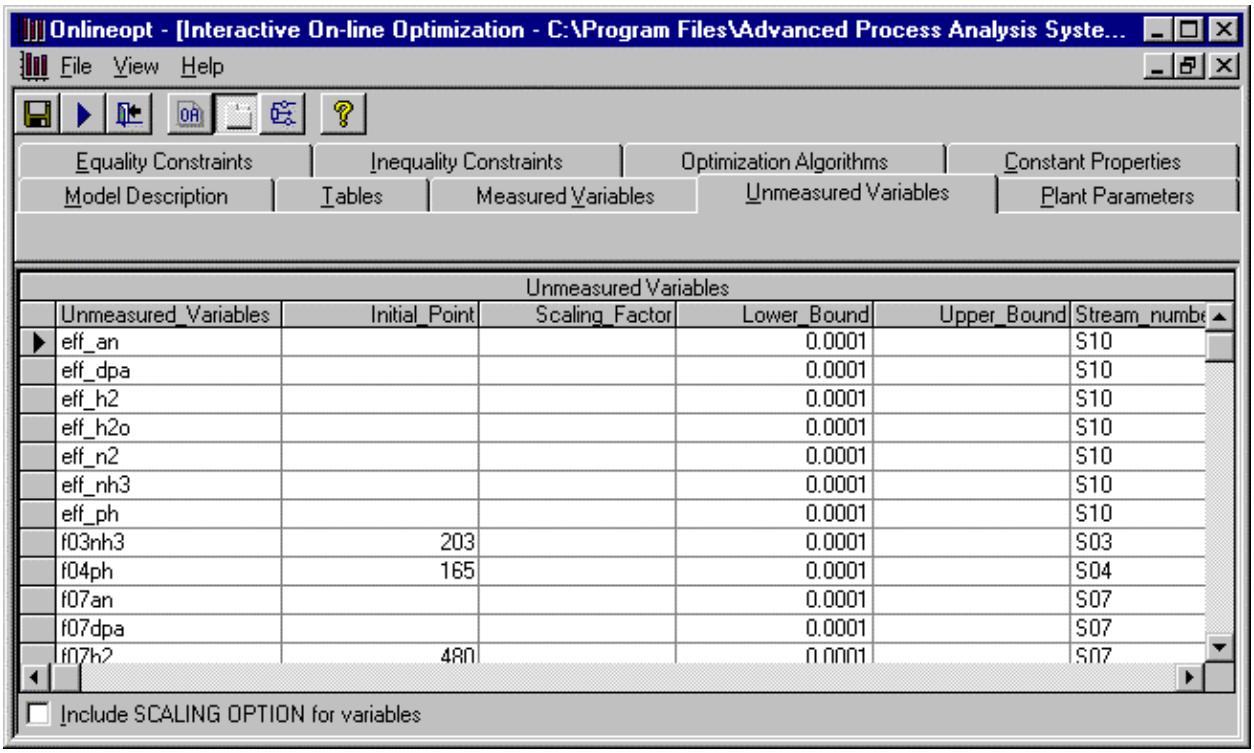
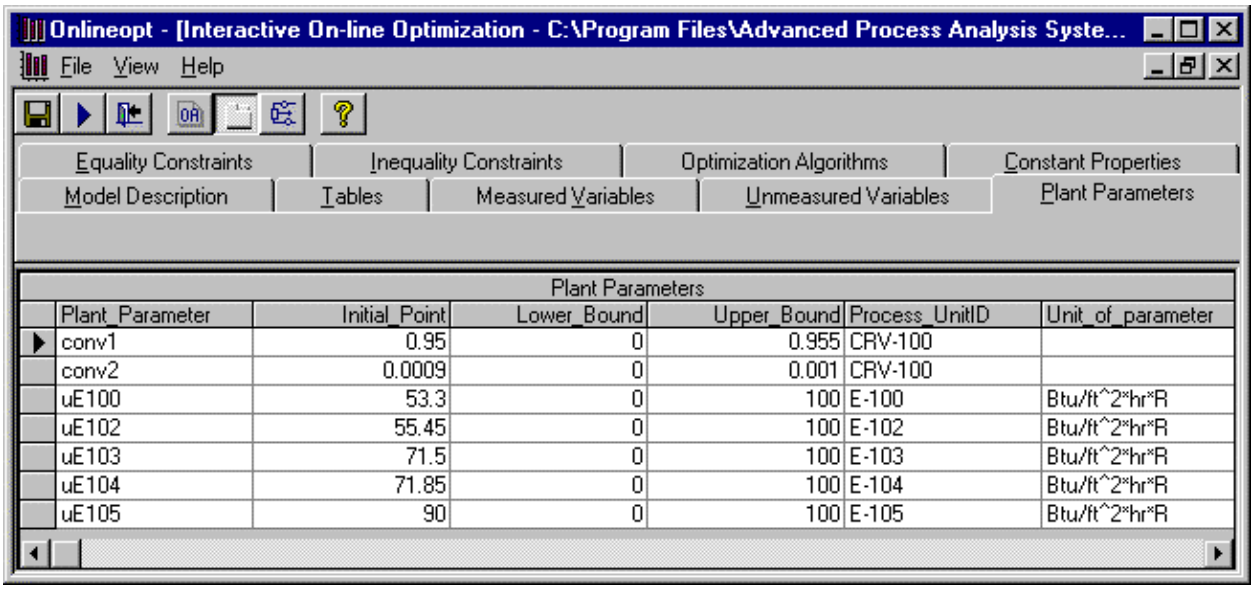


Figure 40: Unmeasured Variables Window

Let us proceed to the Plant Parameters window by clicking on the 'Plant Parameters' tab. The Plant Parameters window lists all the parameters entered in the Unit and the Global Data window of the FlowSim program. The Plant Parameters window is shown in Figure 41.

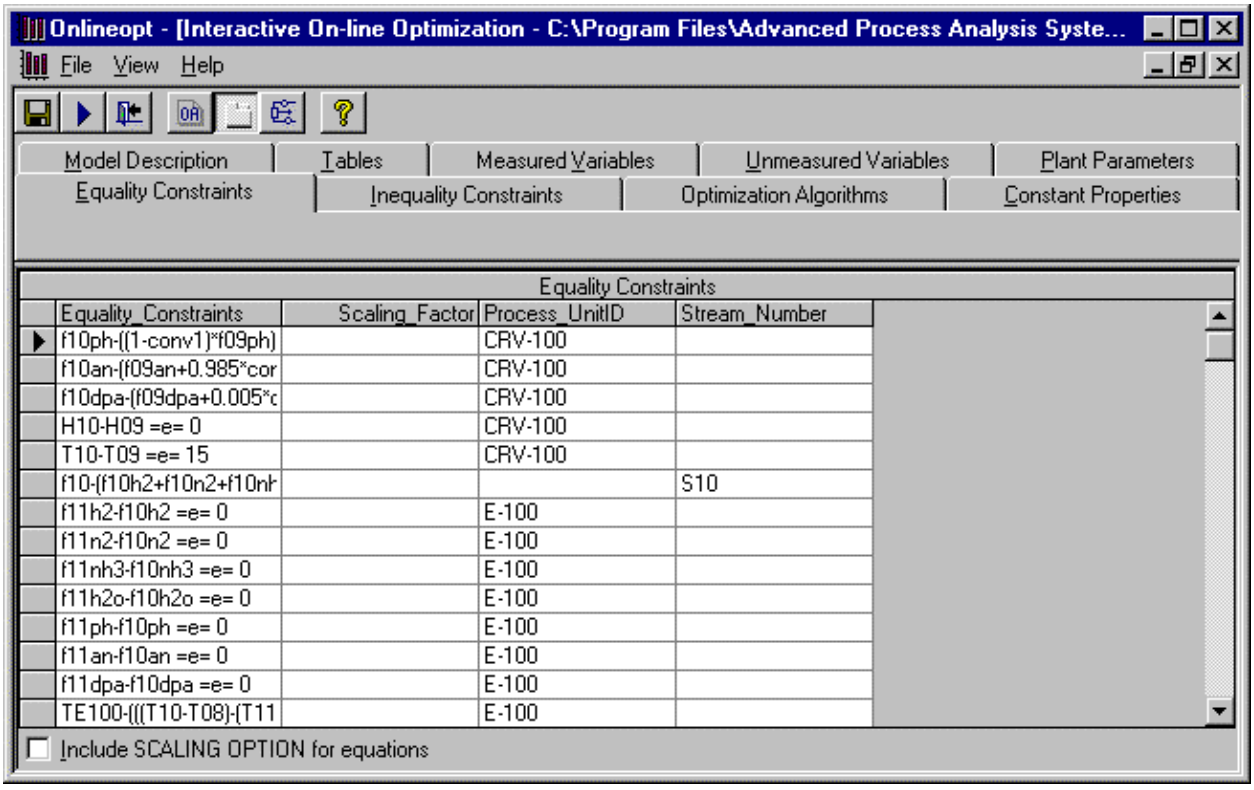
Then proceed to the Equality Constraints window. This window has four columns for displaying the constraints, scaling factor, process unitID and stream number. All of the equality constraints entered in the FlowSim program are listed in this window. The Equality Constraints window is shown in Figure 42. The next step is the Inequality Constraints window, which is similar to the Equality Constraints window. The Inequality Constraints window has three columns for displaying the constraints, process unitID and stream number. Scaling factors are not available for inequality constraints.



Plant Parameters

Plant_Parameter	Initial_Point	Lower_Bound	Upper_Bound	Process_UnitID	Unit_of_parameter
conv1	0.95	0	0.955	CRV-100	
conv2	0.0009	0	0.001	CRV-100	
uE100	53.3	0	100	E-100	Btu/ft^2*hr*R
uE102	55.45	0	100	E-102	Btu/ft^2*hr*R
uE103	71.5	0	100	E-103	Btu/ft^2*hr*R
uE104	71.85	0	100	E-104	Btu/ft^2*hr*R
uE105	90	0	100	E-105	Btu/ft^2*hr*R

Figure 41. Plant Parameters Window



Equality Constraints

Equality_Constraints	Scaling_Factor	Process_UnitID	Stream_Number
f10ph-((1-conv1)*f09ph)		CRV-100	
f10an-(f09an+0.985*cor		CRV-100	
f10dpa-(f09dpa+0.005*c		CRV-100	
H10-H09 =e= 0		CRV-100	
T10-T09 =e= 15		CRV-100	
f10-(f10h2+f10n2+f10nh			S10
f11h2-f10h2 =e= 0		E-100	
f11n2-f10n2 =e= 0		E-100	
f11nh3-f10nh3 =e= 0		E-100	
f11h2o-f10h2o =e= 0		E-100	
f11ph-f10ph =e= 0		E-100	
f11an-f10an =e= 0		E-100	
f11dpa-f10dpa =e= 0		E-100	
TE100-(((T10-T08)-(T11		E-100	

Include SCALING OPTION for equations

Figure 42.Equality Constraints Window

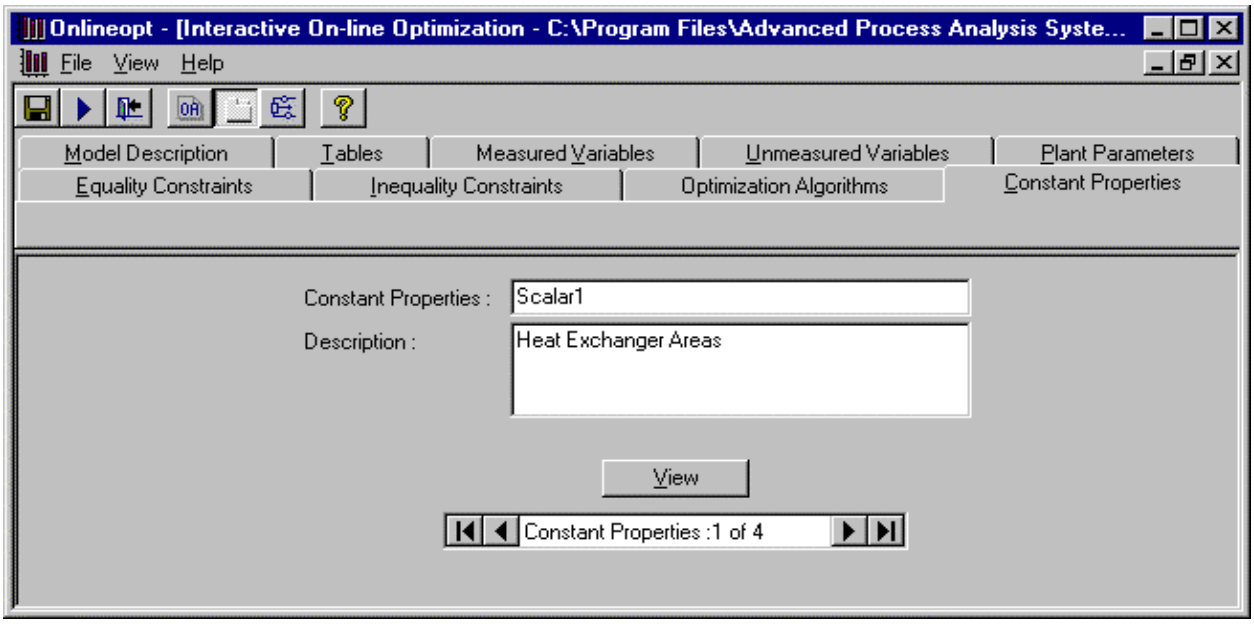


Figure 43. Constant Properties Window

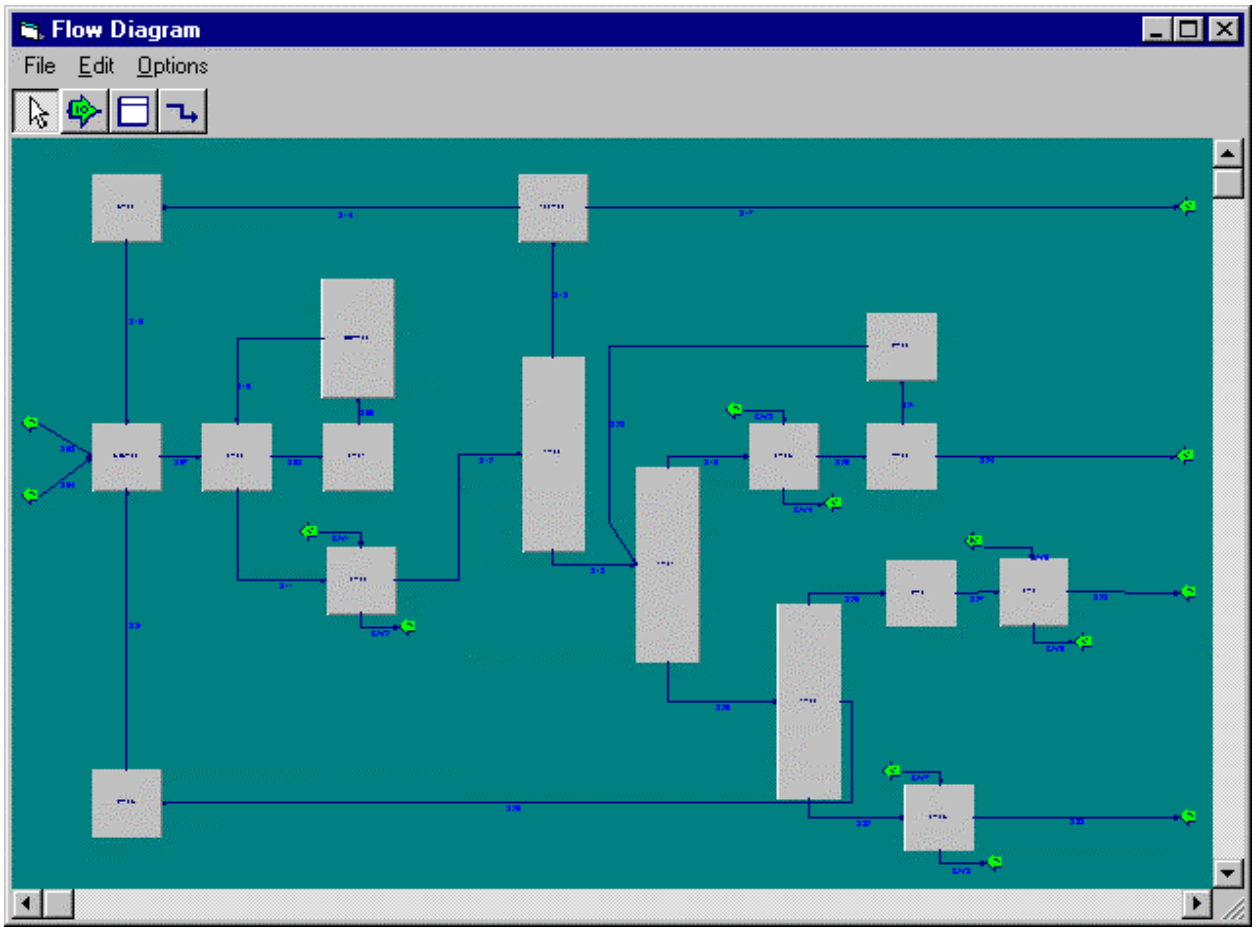


Figure44. Flowsheet Diagram Window

The next step is the Constant Properties window. The constant properties window is shown in Figure 42.

The flowsheet diagram can be viewed by clicking on the 'FlowSheet Diagram' option in the view menu as shown in Figure 36. The flowsheet cannot be edited in the On-line Optimization program. The flowsheet diagram is shown in Figure 44. Double clicking on a unit opens a data form which displays all the measured variables, unmeasured variables and plant parameters that are associated with that unit. Similarly, double clicking on a stream opens a data form which displays the measured and unmeasured variables, associated with the stream. The global data can be viewed by double clicking on the background of the flowsheet

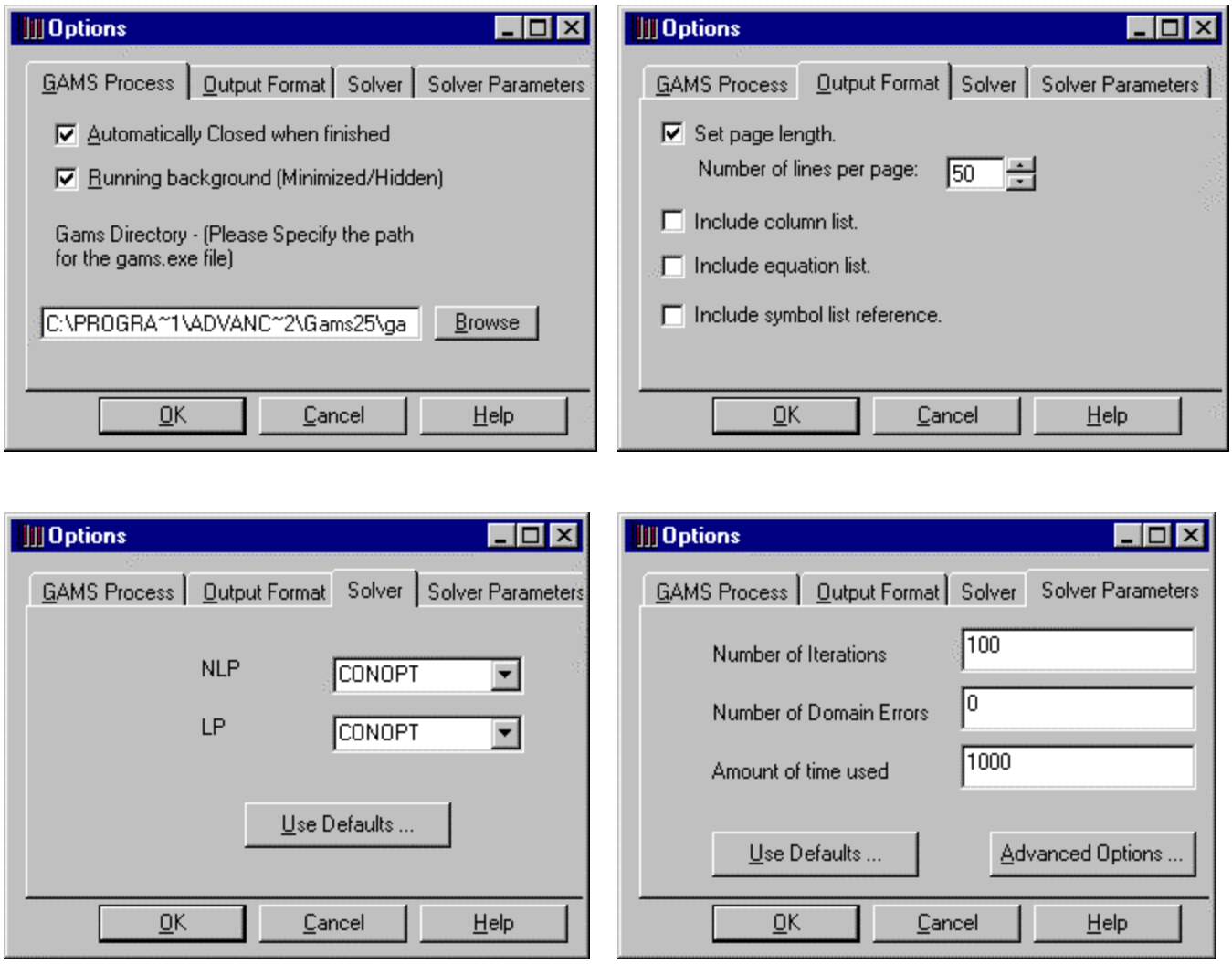


Figure 45. Options With **GAMS** process tab

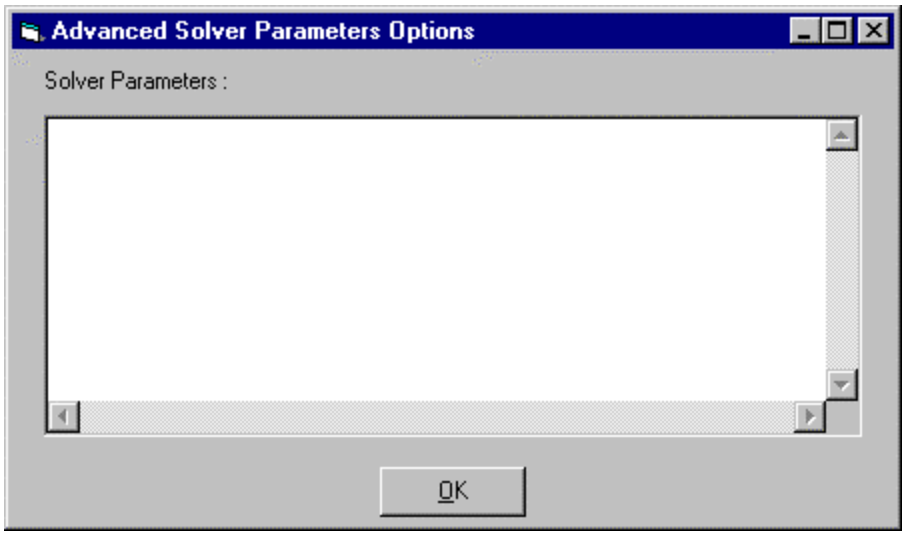


Figure 46. Advanced Parameters Options Window

Clicking on the 'Options' item in 'View' menu, opens the Options window as shown in Figure 45. General GAMS Process options are set in the 'GAMS Process' tab as shown in the first window of Figure 45. The format for the GAMS output can be specified in the 'Output Format' tab as shown in second window of Figure 45. LP and NLP values for the Solver can be set in the 'Solver' tab as shown in the third window of Figure 45. The default values are CONOPT for both LP and NLP. These default values can be restored by clicking on the 'Use Defaults…' button. Solver Parameters like Number of Iterations, Number of Domain Errors and Amount of Time Used can be specified in the 'Solver Parameters' tab as shown in the fourth window of Figure 45. The recommended values for the 'Solver Parameters' of the aniline process are Number of iterations 100, Domain Errors 0, and Amount of time Used 1000 sec. The default values for Number of iterations 1000, Number of Domain Errors 0, and Amount of time used 1000 sec can be restored by clicking on the 'Use Defaults…' button. Other advanced options can be set by clicking on the 'Advanced Options' button, which brings up the window shown in Figure 46.

After entering the required information, let us proceed to execute the model. To execute the model, click on the 'Execute' option in the File menu or click on the 'Execute' button (the button with the triangle) in the toolbar. Once the 'Execute' option is clicked the Model Summary and Execute window as shown in Figure 47 is opened. This window gives the summary of the aniline process.

When the 'Execute' button in the 'Model Execute and Summary' window is clicked, the program first extracts the model information from the database. Based on this information, it generates the GAMS input files and calls the GAMS solver. The progress of the GAMS program execution is shown in Figure 48. This window is automatically closed as soon as the execution is over. When the execution of the program is completed, it displays the results of the on-line optimization in the Output window.

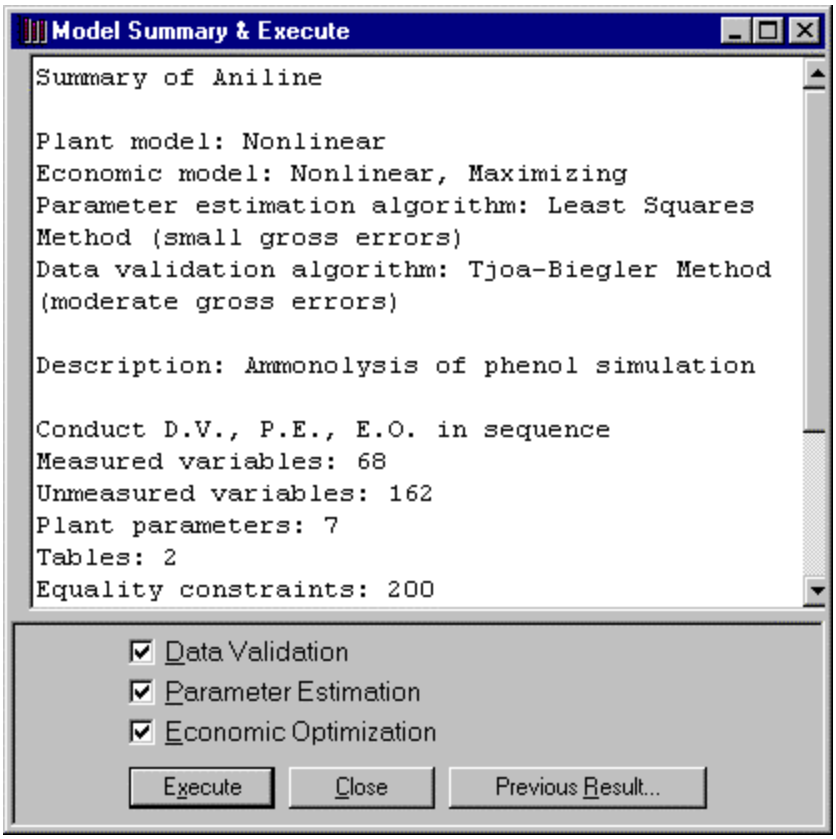


Figure 47. Model Execution Summary Window

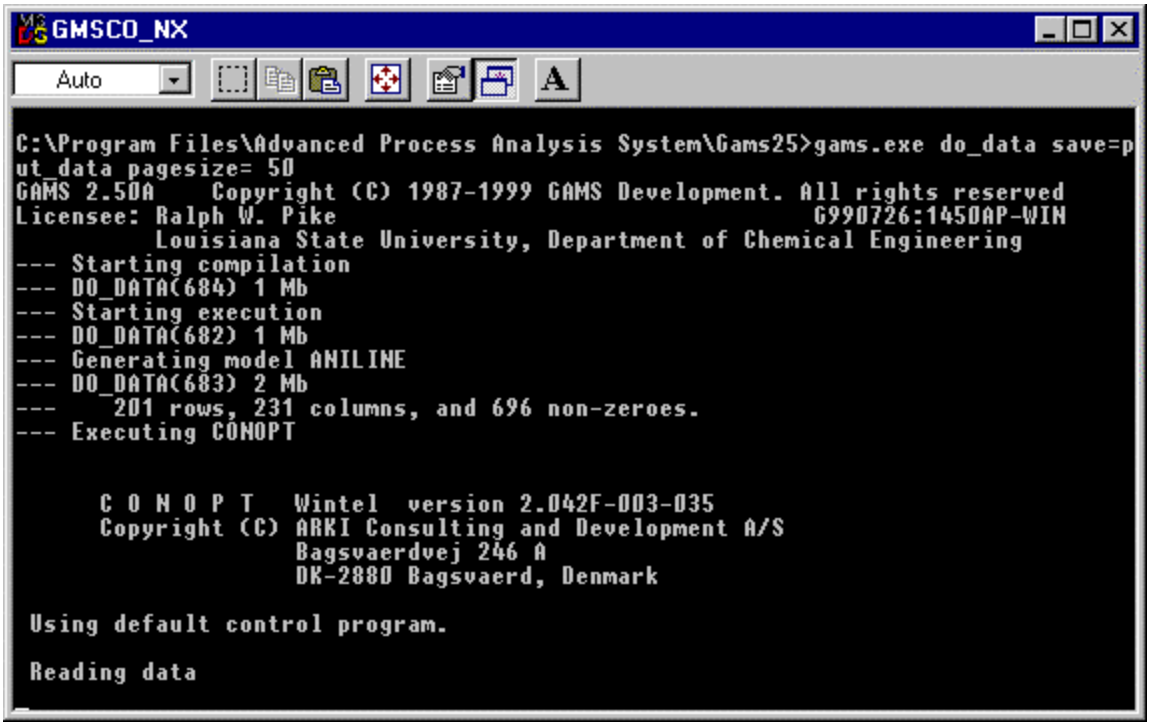

GMSCO_NX
Auto
C:\Program Files\Advanced Process Analysis System\Gams25>gams.exe do_data save=p
ut_data pagesize= 50
GAMS 2.50A Copyright (C) 1987-1999 GAMS Development. All rights reserved
Licensee: Ralph W. Pike G990726:145DAP-WIN
Louisiana State University, Department of Chemical Engineering
--- Starting compilation
--- DO_DATA(684) 1 Mb
--- Starting execution
--- DO_DATA(682) 1 Mb
--- Generating model ANILINE
--- DO_DATA(683) 2 Mb
--- 201 rows, 231 columns, and 696 non-zeroes.
--- Executing CONOPT
C O N O P T Wintel version 2.042F-003-035
Copyright (C) ARKI Consulting and Development A/S
Bagsvaerdvej 246 A
DK-2880 Bagsvaerd, Denmark
Using default control program.
Reading data

Figure 48.**GAMS** Program Execution Window

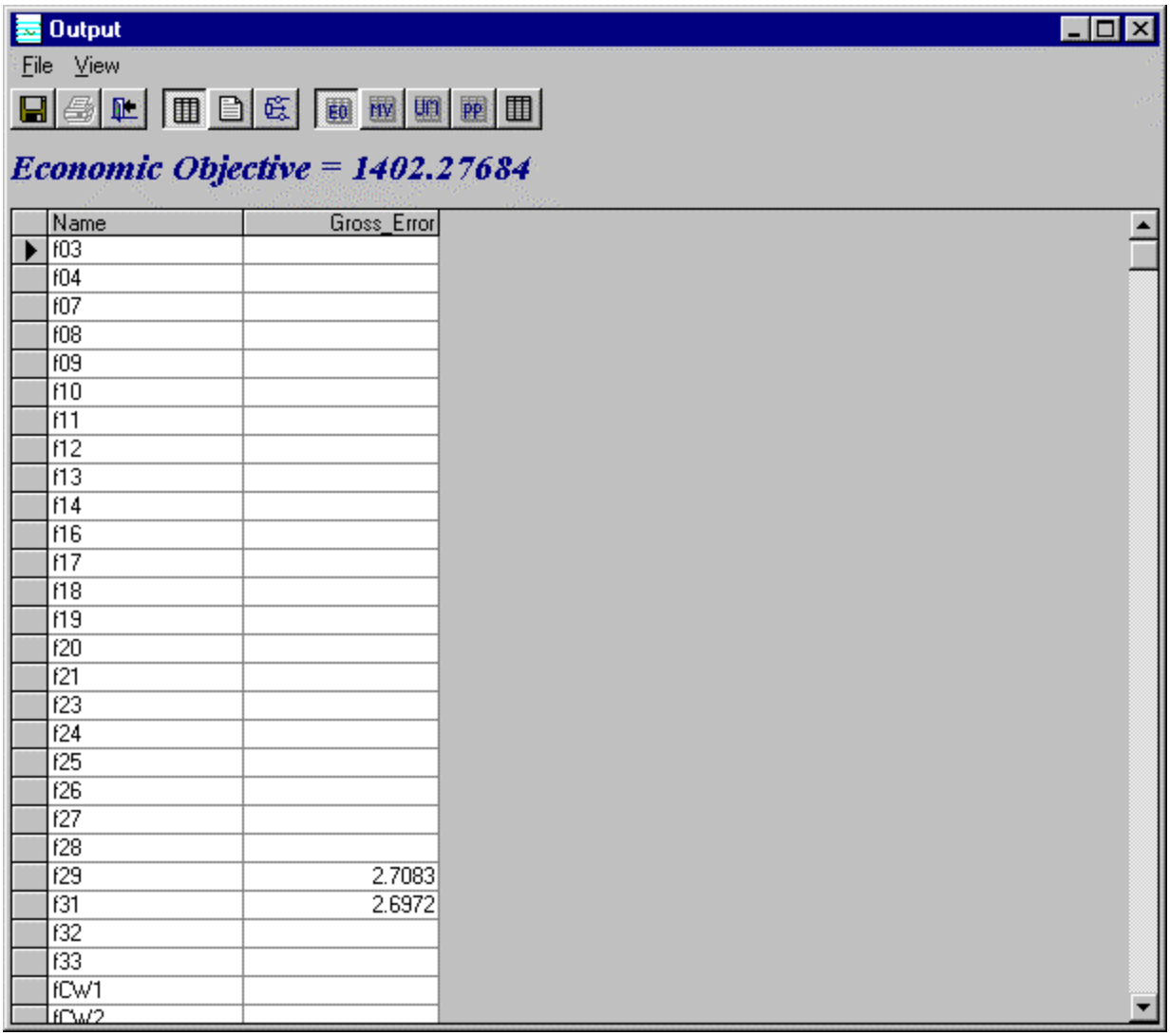


Figure 49. Final Report in the Output Window

After the three programs have been executed, three detailed GAMS output files will be generated by GAMS for the three optimization problems. These files give detailed solutions of the optimization problems for Data Validation, Parameter Estimation and Economic Optimization. Also, a final report is generated by the Interactive On-line Optimization system. In the final report, the estimated values of the parameters, the reconciled values of process variables, the optimal set points and the profit from Economic Optimization are shown. The Output Window with the Final Report is shown in Figure 49. The View menu in the Output window has three options named Final Report, Full Output and Flowsheet.

The Final Report option has five options namely the Economic Objective, the Measured Variables, the Unmeasured Variables, the Plant Parameters and the Stream Number as shown in Figure 50. The Economic Objective value is shown in Figure 49.

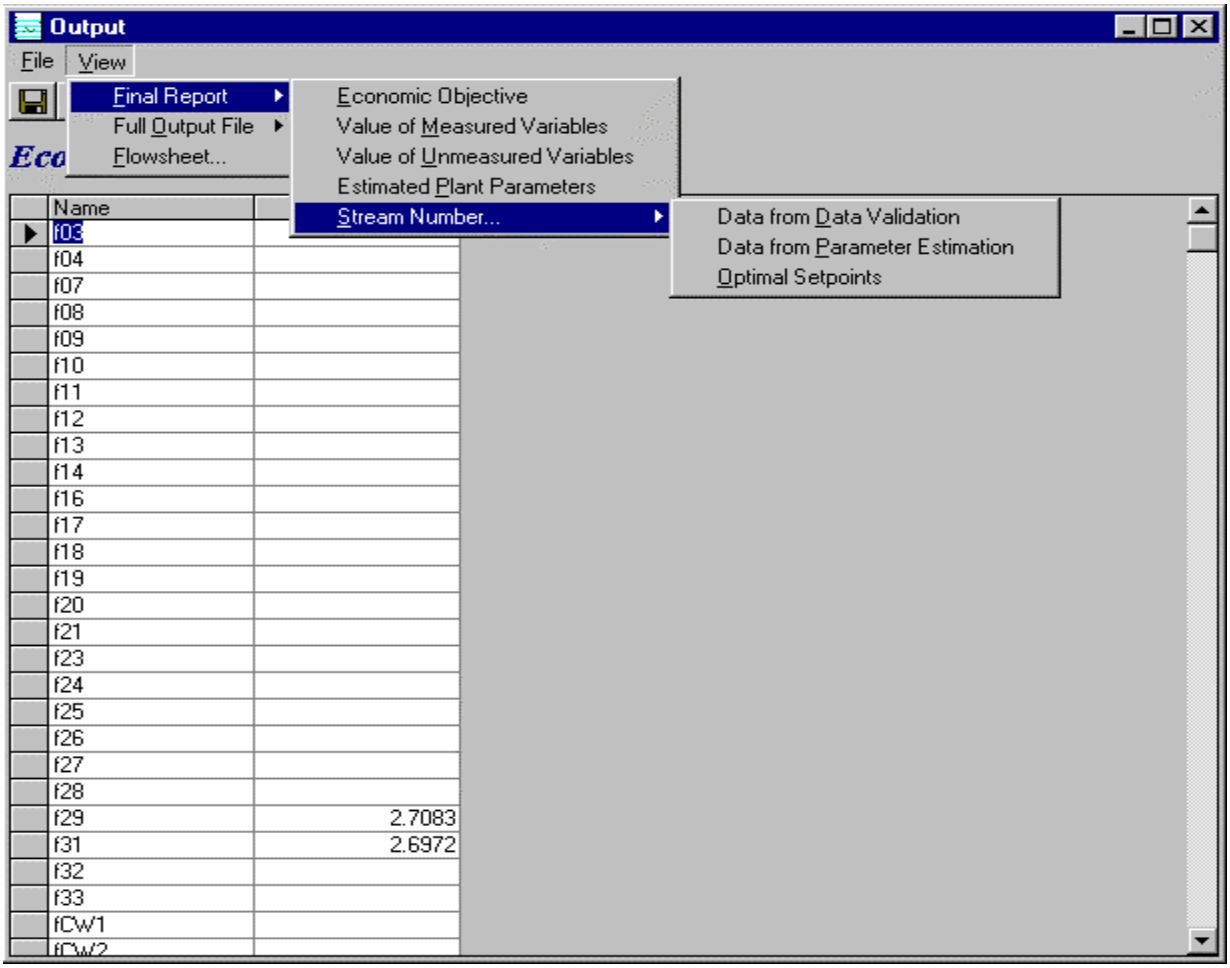
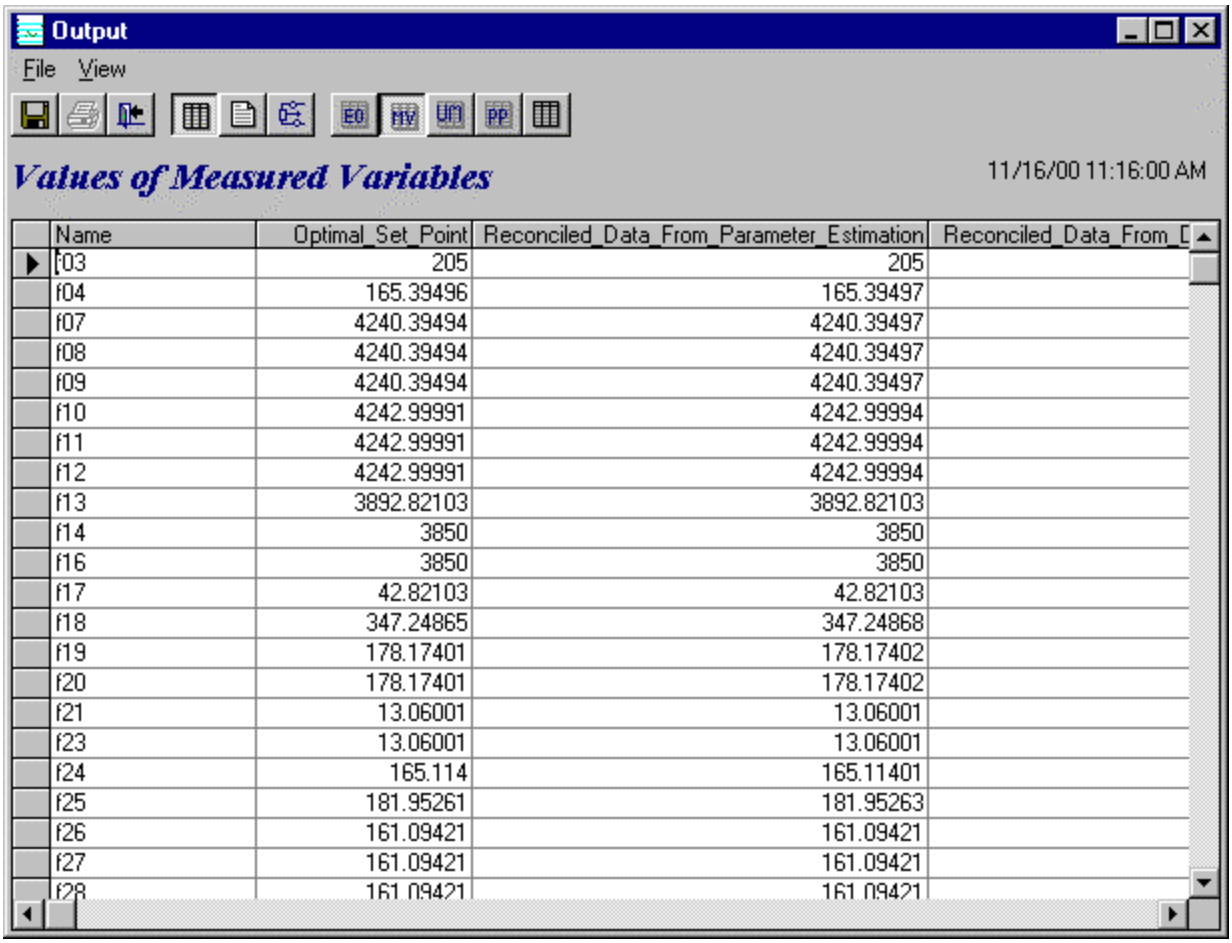


Figure 50: View Menu in the output Window

When the option 'Measured Variables' in the Final Report menu is clicked, the system opens a spreadsheet data form which includes the optimal setpoints from economic optimization, reconciled values from Data Validation, reconciled values from Parameter Estimation and the plant data as shown in Figure 51. Clicking on "Plant Parameters" in the Final Report menu, the system opens a spreadsheet data form that includes the estimated values of plant parameters as shown in Figure 52.

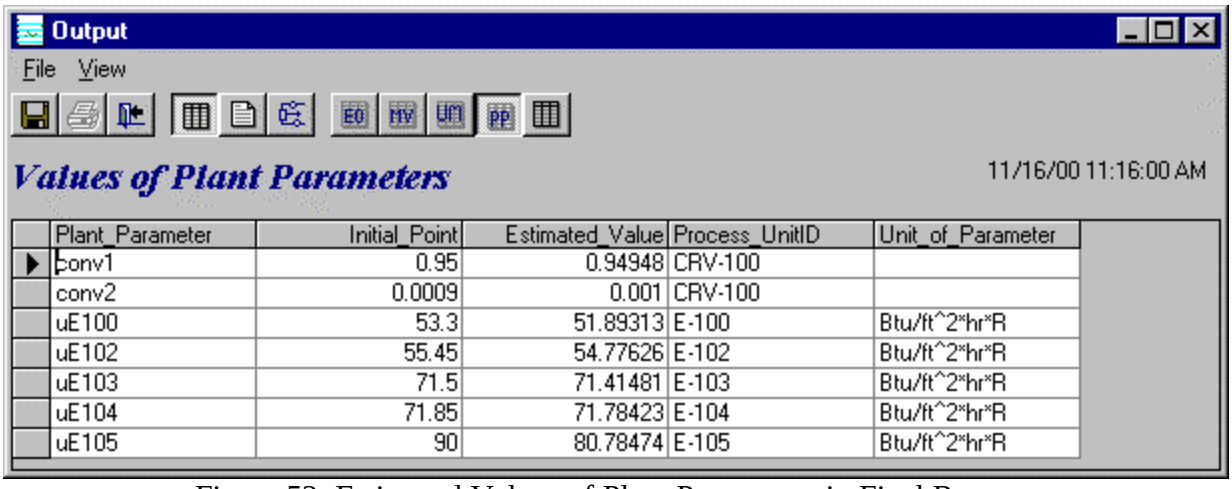
Clicking on the "Unmeasured Variables", the system opens a spreadsheet data form which includes the unmeasured variables and their reconciled values as shown in Figure 53.

Three options are available in the 'Stream Number' menu as shown in Figure 50. The three options are Data from Data Validation, Data from Parameter Estimation and Optimal Setpoints. Let us click the 'Data from Data Validation' option. An input box appears. Let us enter 's07' and click 'Ok'. The Measured Variables and Unmeasured variables which are associated with the stream 's07' with their reconciled values from Data Validation are displayed as shown in Figure 54.



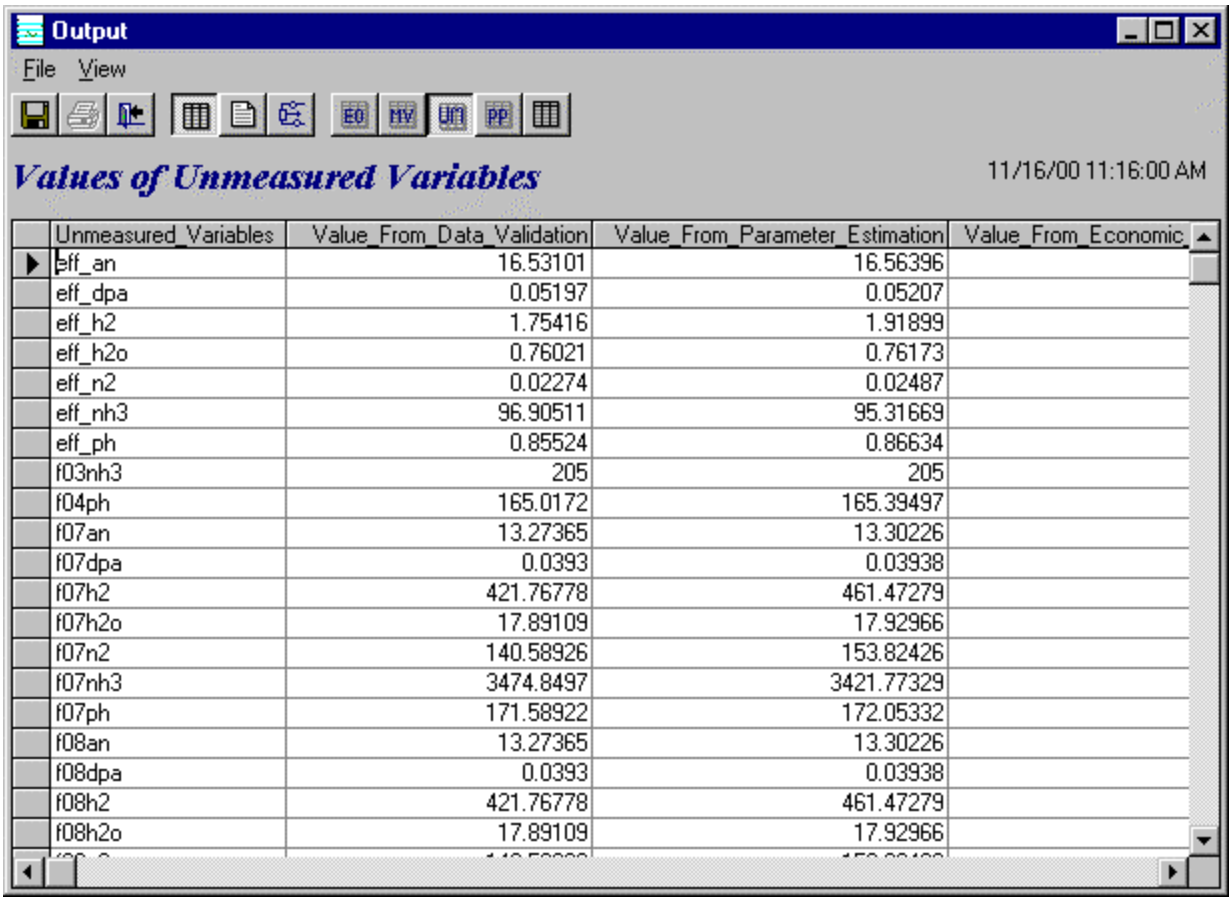
Name	Optimal_Set_Point	Reconciled_Data_From_Parameter_Estimation	Reconciled_Data_From_D
f03	205	205	
f04	165.39496	165.39497	
f07	4240.39494	4240.39497	
f08	4240.39494	4240.39497	
f09	4240.39494	4240.39497	
f10	4242.99991	4242.99994	
f11	4242.99991	4242.99994	
f12	4242.99991	4242.99994	
f13	3892.82103	3892.82103	
f14	3850	3850	
f16	3850	3850	
f17	42.82103	42.82103	
f18	347.24865	347.24868	
f19	178.17401	178.17402	
f20	178.17401	178.17402	
f21	13.06001	13.06001	
f23	13.06001	13.06001	
f24	165.114	165.11401	
f25	181.95261	181.95263	
f26	161.09421	161.09421	
f27	161.09421	161.09421	
f28	161.09421	161.09421	

Figure 51: Optimal Set points and Reconciled Data in Final Report for Measured Variables



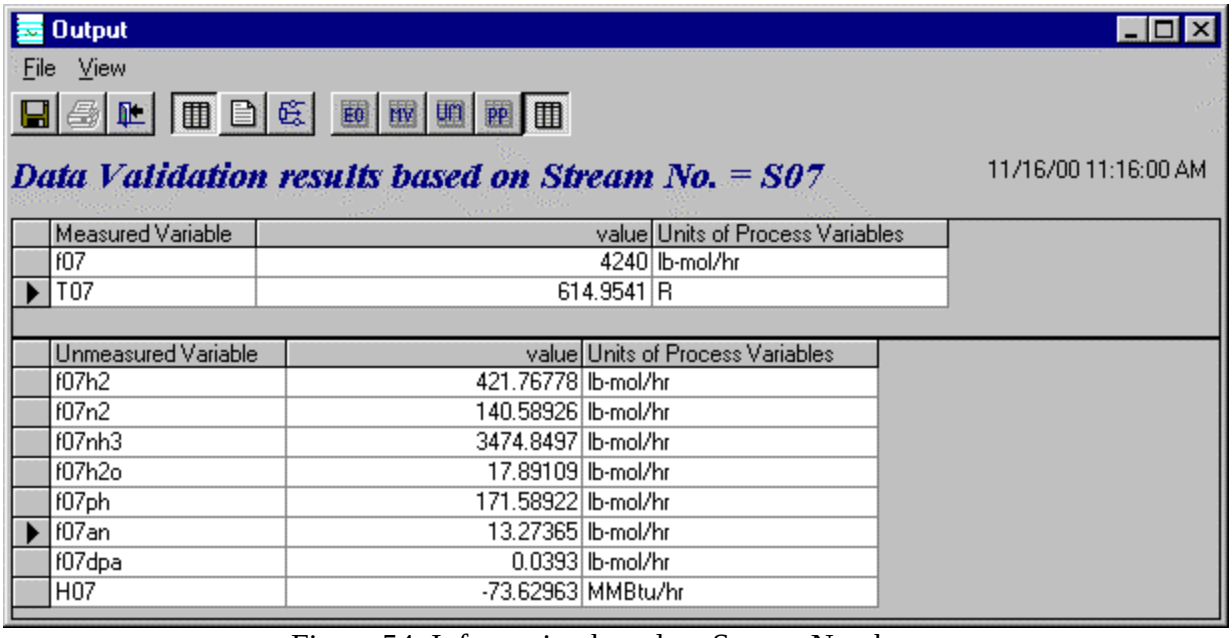
Plant_Parameter	Initial_Point	Estimated_Value	Process_UnitID	Unit_of_Parameter
conv1	0.95	0.94948	CRV-100	
conv2	0.0009	0.001	CRV-100	
uE100	53.3	51.89313	E-100	Btu/ft^2*hr*R
uE102	55.45	54.77626	E-102	Btu/ft^2*hr*R
uE103	71.5	71.41481	E-103	Btu/ft^2*hr*R
uE104	71.85	71.78423	E-104	Btu/ft^2*hr*R
uE105	90	80.78474	E-105	Btu/ft^2*hr*R

Figure 52: Estimated Values of Plant Parameters in Final Report



Unmeasured_Variables	Value_From_Data_Validation	Value_From_Parameter_Estimation	Value_From_Economic
eff_an	16.53101	16.56396	
eff_dpa	0.05197	0.05207	
eff_h2	1.75416	1.91899	
eff_h2o	0.76021	0.76173	
eff_n2	0.02274	0.02487	
eff_nh3	96.90511	95.31669	
eff_ph	0.85524	0.86634	
f03nh3	205	205	
f04ph	165.0172	165.39497	
f07an	13.27365	13.30226	
f07dpa	0.0393	0.03938	
f07h2	421.76778	461.47279	
f07h2o	17.89109	17.92966	
f07n2	140.58926	153.82426	
f07nh3	3474.8497	3421.77329	
f07ph	171.58922	172.05332	
f08an	13.27365	13.30226	
f08dpa	0.0393	0.03938	
f08h2	421.76778	461.47279	
f08h2o	17.89109	17.92966	

Figure 53: Reconciled Values for Unmeasured Variables



Measured Variable	value	Units of Process Variables
f07	4240	lb-mol/hr
T07	614.9541	R

Unmeasured Variable	value	Units of Process Variables
f07h2	421.76778	lb-mol/hr
f07n2	140.58926	lb-mol/hr
f07nh3	3474.8497	lb-mol/hr
f07h2o	17.89109	lb-mol/hr
f07ph	171.58922	lb-mol/hr
f07an	13.27365	lb-mol/hr
f07dpa	0.0393	lb-mol/hr
H07	-73.62963	MMBtu/hr

Figure 54: Information based on Stream Number

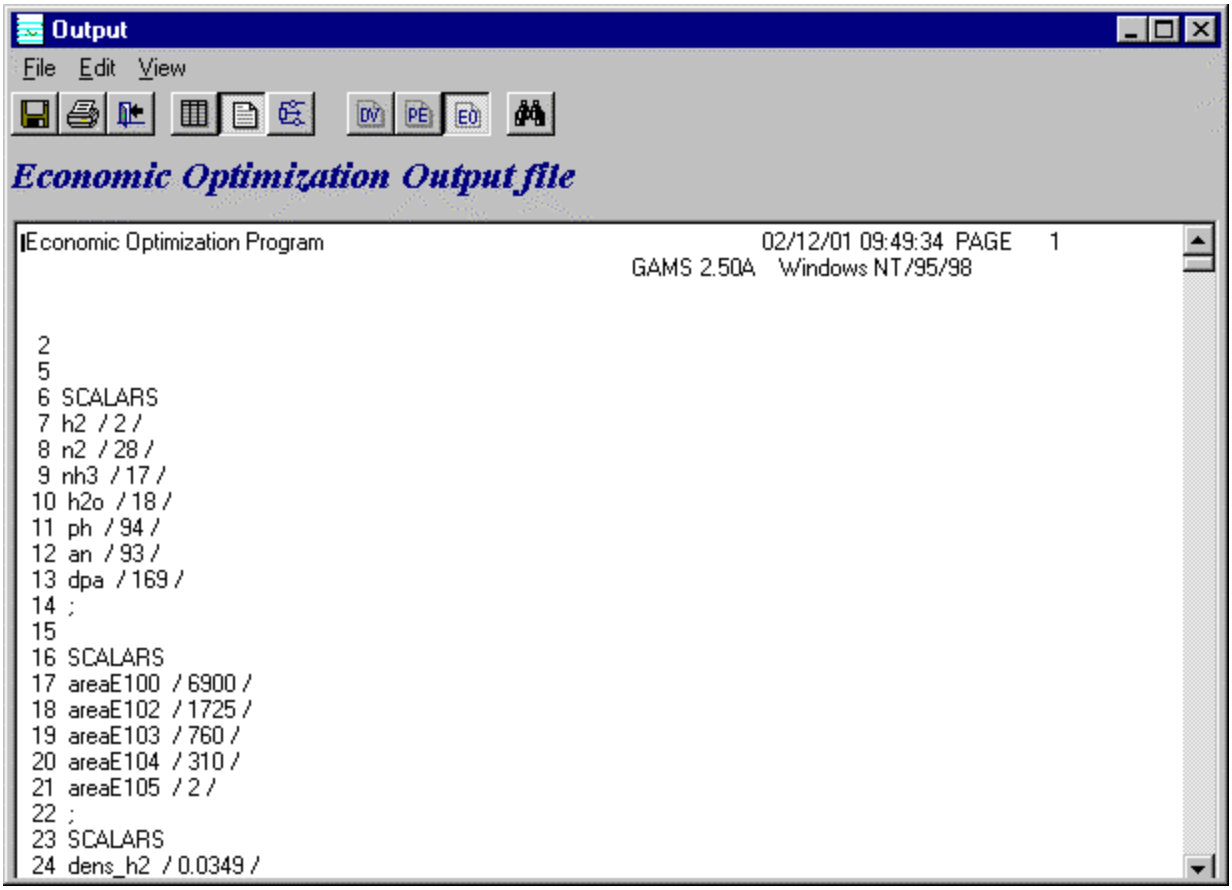


Figure 55. Full Output File of GAMS Programs

When the 'Full Output File' option in the view menu is selected, three buttons are displayed in the toolbar each corresponding to the three optimization problems. Clicking a button will open the corresponding output file for viewing. Let us click on the 'Data Validation' option in the Full Output menu. The full output file is shown in Figure 55.

The user can use the 'Find' and 'Goto' options in the Edit menu to search for a particular phrase or go to a particular section in the Full Output file. The Final Report can be exported as an Excel file using the 'Export' option in the file menu. The Full Output files can also be exported as a text file using the 'Export' option.

The results can also be viewed as a flowsheet in a window similar to the one shown in Figure 44. Double clicking on a stream or unit opens the corresponding data window. The Data window for stream 's07' is shown in Figure 56. As seen in this figure, the values of the measured variables obtained as a result of on-line optimization are displayed in the data window.

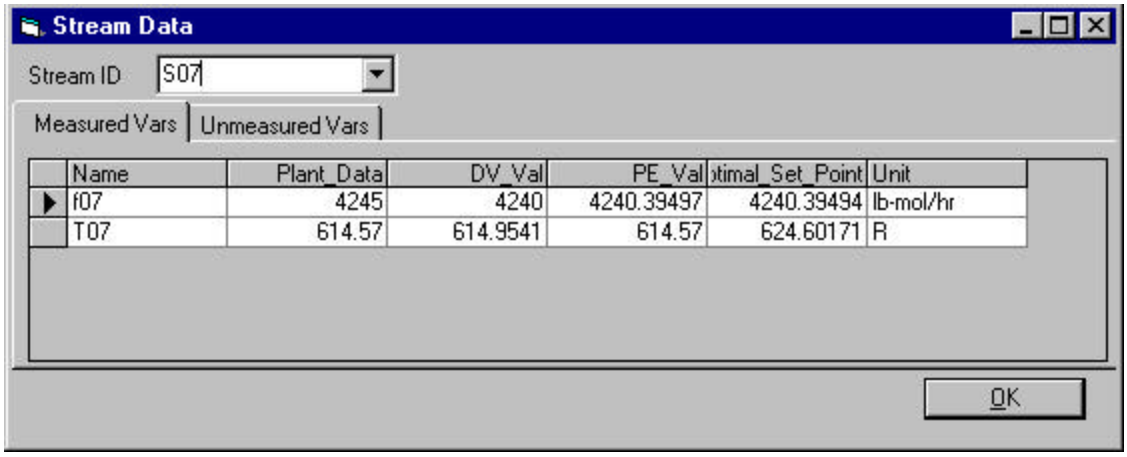


Figure 56: Stream Data Window

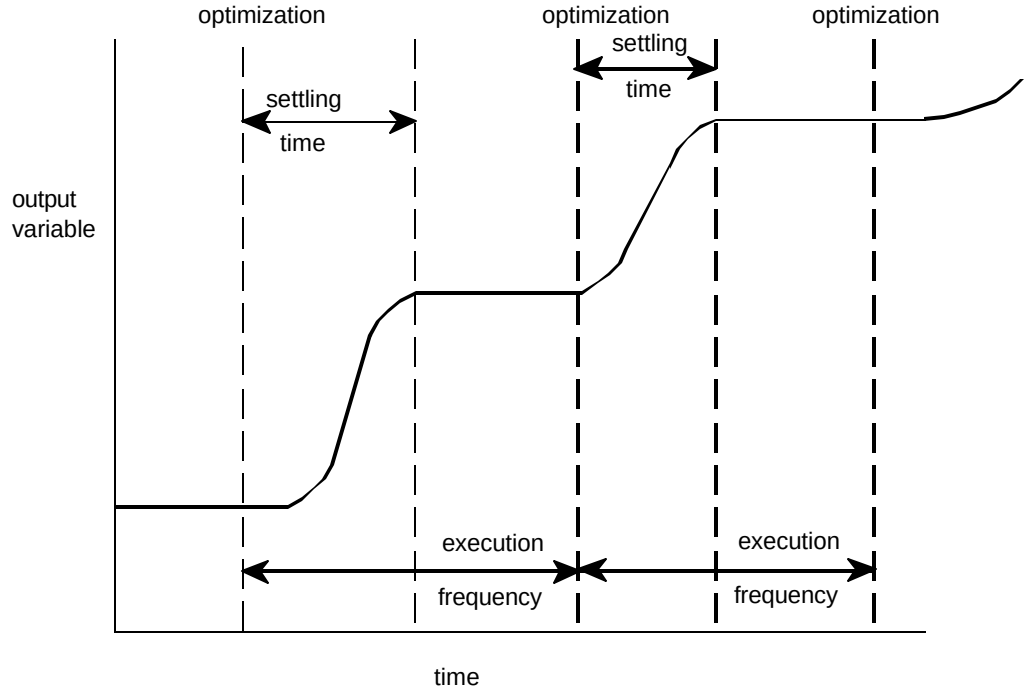
Clicking the 'Close' option in the file menu of the Output window returns the user to the main screen, which was shown in Figure 35. The model information can be exported as an Excel file using the 'Export' option in the file menu of the main window. Save the optimization results using the 'Save' option in the file menu. The results including the full output files are stored along with the model. When the 'Exit' button is clicked, the Interactive On-line Optimization main window is closed and the user is taken back to the Advanced Process Analysis Desk.

Steady-State Detection and Execution Frequency

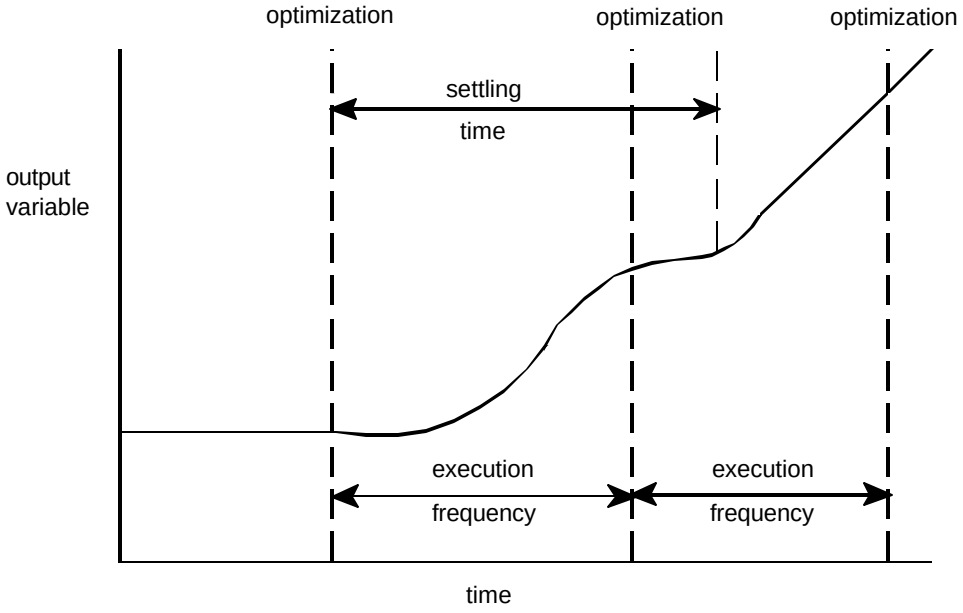
On-line optimization executes economic optimization and generates a set of optimal set points. Then these set points are transferred to the coordinator program or the operators as an Excel spreadsheet file. These optimal set points can either be sent directly to the distributed control system or viewed by operators before they are sent to the DCS. Before the optimal set points are implemented, the steady state detection program is run to ensure the process is at steady state. The following gives detailed information about steady-state detection and execution frequency.

The execution frequency for optimization is the time between conducting on-line optimization of the process, and it has to be determined for each of the units in the process. It depends on the settling time, i.e., the time required for the units in the process to move from one set of steady-state operating conditions to another. This settling time can be estimated from the time constant determined by process step testing. The time period between two on-line optimization executions must be longer than the settling time to ensure that the units have returned to steady state operations before the optimization is conducted again. This is illustrated in Figure 57, after Darby and White (1988). The figure shows that execution frequency for optimization in Figure 57-a was satisfactory for the process, but the execution frequency in Figure 57-b was too rapid for the process. In Figure 57-a, the process has returned to steady-state operations and held that position until the next optimization. However, in Figure 57-b, the process did not have enough time to return to steady-state operations before the optimization altered the operating conditions. The process would continue on an unsteady state path, and

operator intervention would be required. The settling time for an ethylene plant is four hours according to Darby and White (1988), and this time for the sulfuric acid contact process is twelve hours according Hertwig (1997).



a. Time between optimizations is longer than settling time



b. Time between optimizations is less than settling time

Figure57. Comparison of Time between Optimizations and Process Settling Time after Darby and White

As shown in Figure 57, it is necessary to make sure that the process is operating at steady state before the plant data is taken from distributed control system for conducting on-line optimization. Steady state plant data is required for steady state process models.

The time series horizontal screening method has been used in industry to detect a steady state. In this method, the measured values for key process variables are observed for a time period. If the measured values remain within the bounds of two standard deviations, then the process is said to be operating at steady state. This requires the use of a coordinator program or operator action for identifying steady state and exchanging data between the on-line optimization program and the distributed control system. Excel spreadsheet files are widely used to transfer the data. The use of an Excel spreadsheet is the industry standard way of selecting data and

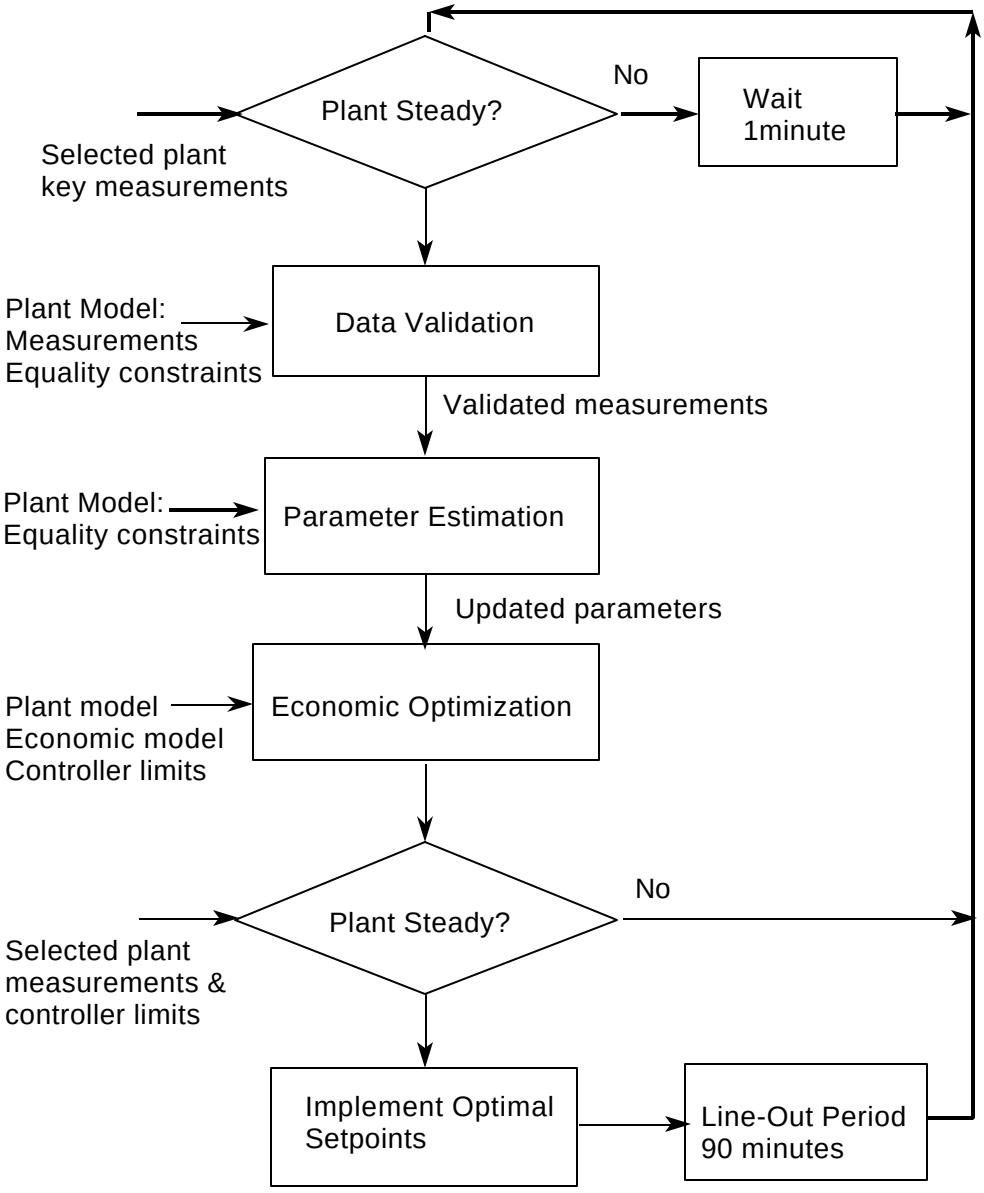


Figure 58. Implementation procedure for On-line Optimization ,after Kelly,et al.(1996)

manipulating data from a DCS. Steady state detection and data exchange will be illustrated with plant data for the contact process.

As shown in Figure 58, on-line optimization executes economic optimization and generates a set of optimal set points. Then these set points are transferred to the coordinator program or the operators as an Excel spreadsheet file. These optimal set points can be sent directly to the distributed control system or viewed by operators before they are sent to the DCS. Before the optimal set points are implemented, the steady state detection program is run to ensure the process is at steady state.

To incorporate the capability for steady state detection, an Excel worksheet program was prepared, *steady.xls*, and it is included in the files with the on-line optimization program. The aniline process is used to illustrate the use of this program for time series analysis for steady state detection. The first sheet in the Excel program has 20 sets of data randomly generated for the aniline process. This information is shown in Figure 59 for the first 14 of these data sets, and each column represents data for the 68 measured variables that would be taken from the data historian of the distributed control system for 20 time intervals ending with the current time.

The second Excel spreadsheet was prepared to analyze this data to determine a time interval that shows the plant operating at steady state. This spreadsheet is shown in Figure 60, and the graphs and buttons were developed using the Visual Basic capabilities that are part of Excel. In this figure, the time series of four of the measured variables can be viewed at one time. The spreadsheet has the capability of displaying any four of the process variables, and the variables that are plotted can be changed by pulling down the menu on the lower left and selecting a variable to be displayed.After reviewing the data in Figure 60, it can be determined when the plant is at steady state between two time periods. Consequently, the decision is to import the data from the middle point of those two time periods, into the on-line optimization

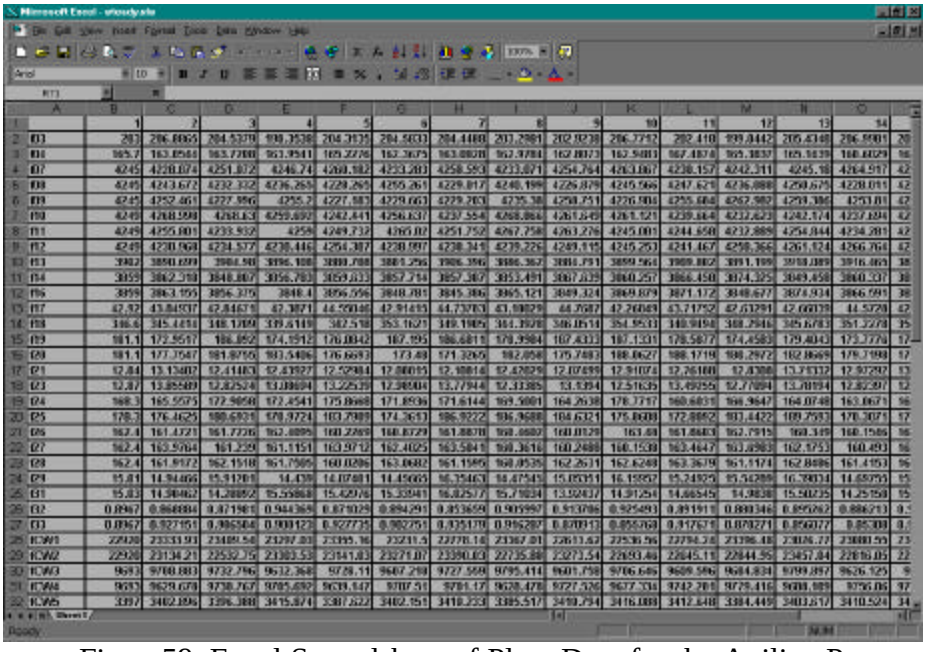


Figure59. Excel Spreadsheet of Plant Data for the Aniline Process

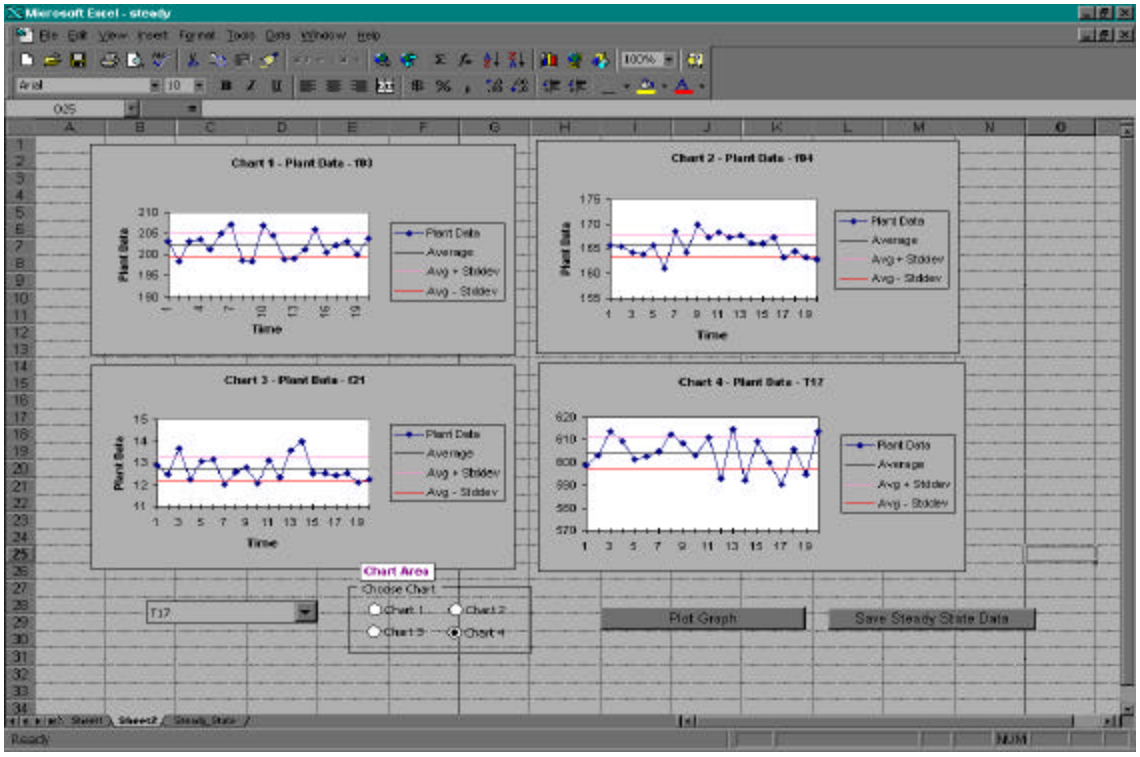


Figure 60. Excel Spreadsheet Showing the Time Series Graphs of the Data

program. On this diagram, the Save Steady State Data button is clicked and the program has the user designate the time interval of the data which is saved to the third spreadsheet, a single column of data that is not shown here as a figure.

The user is now ready to transfer this steady state data to the on-line optimization program. Return to the Declaration Window for Measured Variables, which is shown in Figure 39 and pull down the File menu. This is shown in Figure 61, and then select Import Plant Data. This action brings up the window shown in Figure 62, and in this window the name of the Excel file is designated which contains the steady state plant data that was selected with the Excel time series program. Clicking the Open button will replace the plant data currently in the program. Now having the new data in place, the on-line optimization program can be executed to generate the new set of optimal points for the distributed control system.

The execution of the on-line optimization program generates the set points for the distributed control system. These values can be exported from the on-line optimization program using the same procedure as importing data. The file menu in these windows has a line Export Plant Data which, when clicked, gives a screen similar to the one in Figure 63 to specify the Excel file to transfer this data. The on-line optimization program requires the standard deviation of the measured variables as shown in Figure 39. The Excel program *steady.xls* is used also to calculate the standard deviation of the measured variables. Although not shown in Figure 59, the last column in the spreadsheet is the standard deviation of the measured variables, which was calculated using the 20 measurements. This information can be transferred to the on-line optimization program using the same procedure as was used for the measured variables. However, it is not necessary to use the current plant data to evaluate the standard deviation, and the Excel program can be used with any data set to determine appropriate values of the standard deviation.

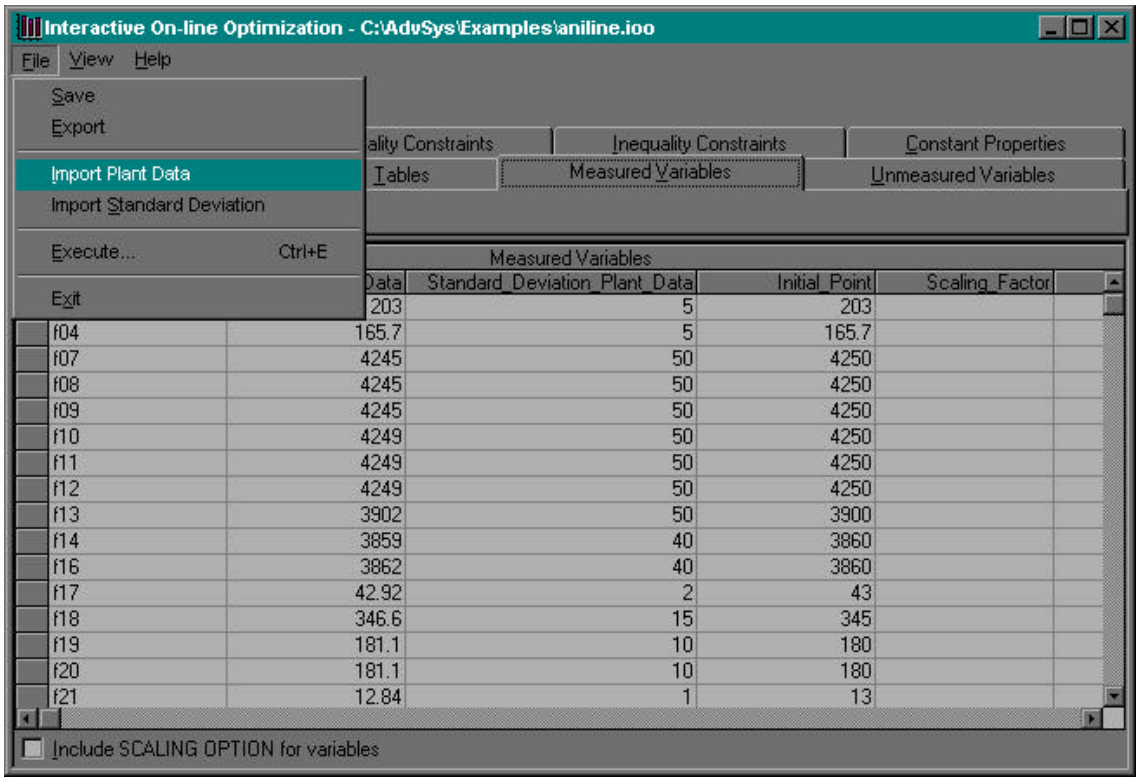


Figure 61. The Import Option in the File menu of On-line Optimization

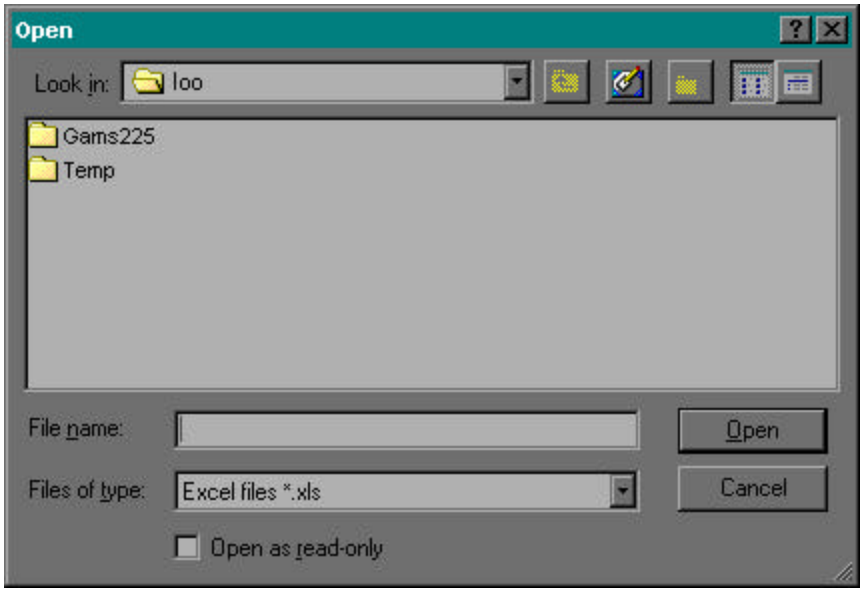


Figure62. The Dialog Box that opens when Import is clicked

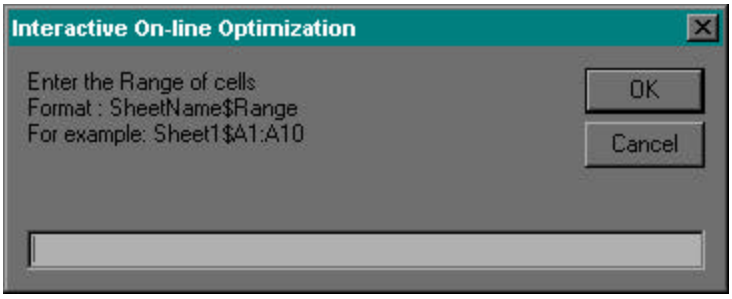


Figure 63. The Screen to enter the Excel Sheet Name and Range

This concludes the description of steady-state detection and execution frequency of on-line optimization. The next step of Advanced Process Analysis System is the heat exchanger network optimization. Click the 'Pinch Analysis' button in Advanced Process Analysis Desk to open the heat exchanger network (THEN) program.

VII. USING THE HEAT EXCHANGER NETWORK (THEN) PROGRAM

Upon clicking the 'Pinch Analysis' button on the Advanced Process Analysis Desk, the 'Heat Exchanger Network Model Information' window is displayed. This window is shown in Figure 64. Since we are using the THEN program for the first time, click the 'New Model' button.

Once the 'Work on Current Model' button is clicked, the 'Welcome Screen' of the Heat Exchanger Network program is displayed. This screen is shown in Figure 65. The message at the center confirms that you are working on the process model 'aniline.ioo' in the 'Examples' subdirectory. The HEN model you are working on is an untitled new model. A HEN model is an input file created by the heat exchanger network program to apply pinch analysis to the process model. A HEN model is stored as a file with a 'hen' extension (e.g. sample.hen).

The menu at the top of the background window is the 'main menu' of THEN. It is available at all times during the execution of the program. The 'Help' button can be used to access online help. The 'About' button gives the copyright information. The 'Exit' button can be used to quit the program at any time and go back to the Advanced Process Analysis Desk.

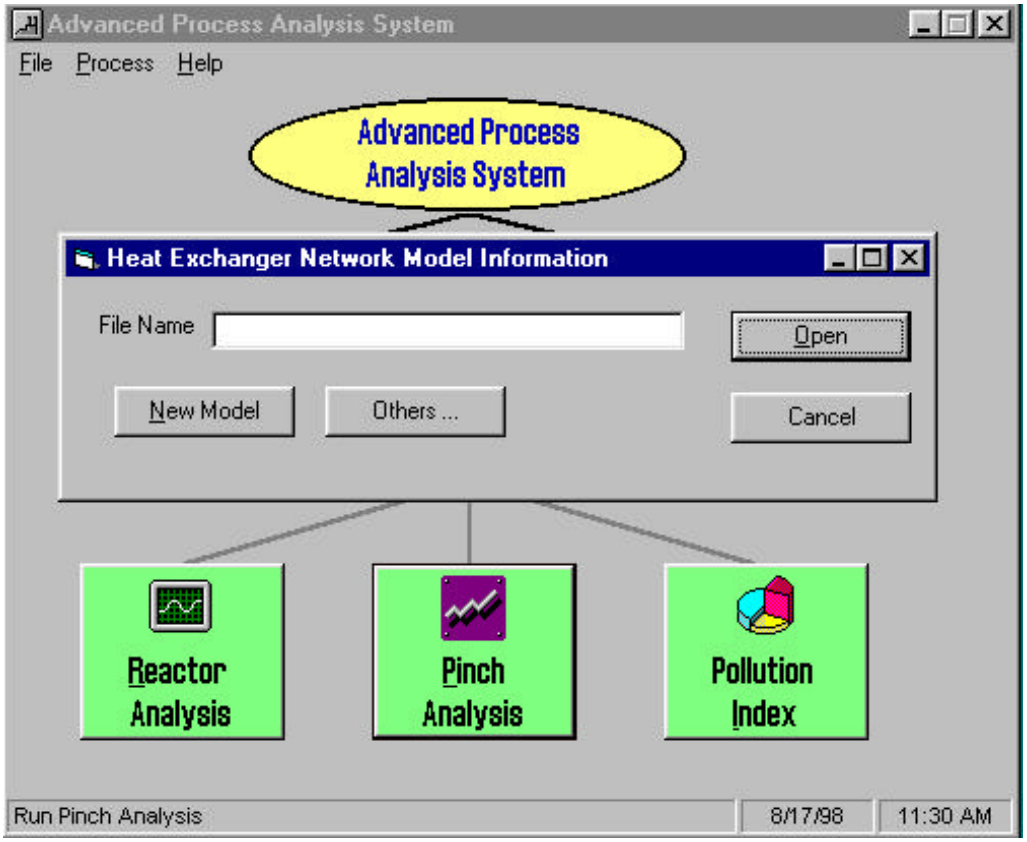


Figure 64 The Heat Exchanger Network Model Information Window

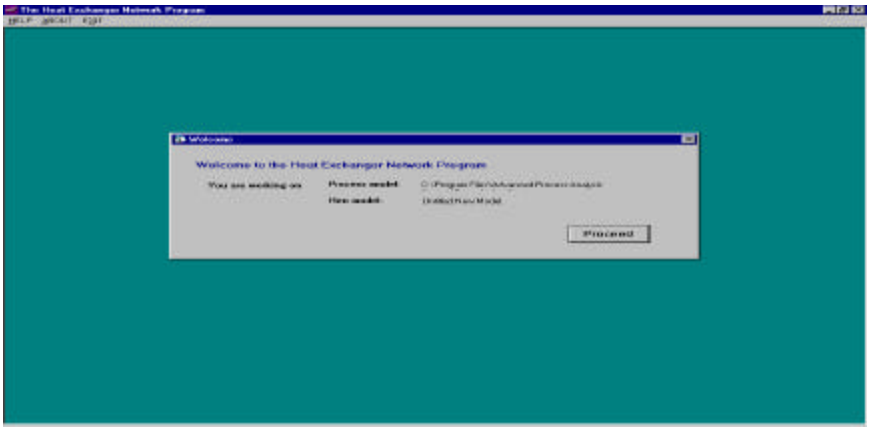


Figure 65. The Welcome Screen THEN.

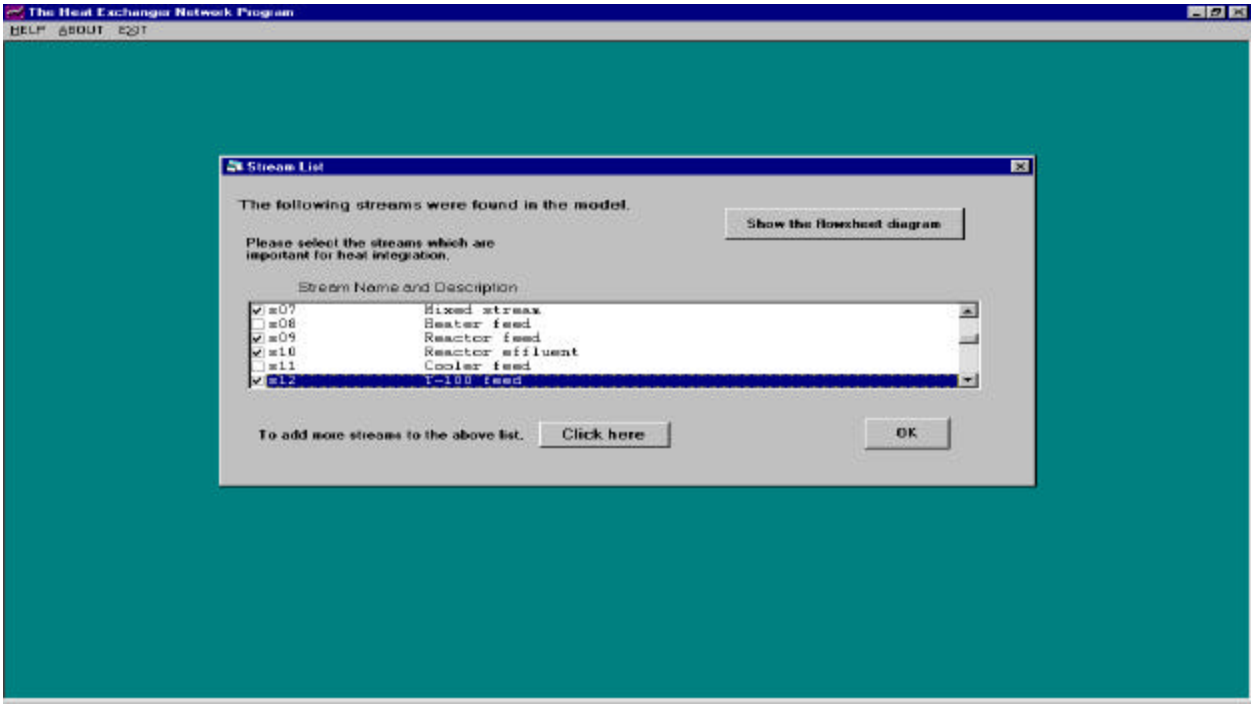

The Heat Exchanger Network Program
HELP ABOUT EXIT
Stream List
The following streams were found in the model.
Show the flowsheet diagram
Please select the streams which are important for heat integration.
Stream Name and Description
s07 Mixed xtmax
s08 Heater feed
s09 Reactor feed
s10 Reactor effluent
s11 Cooler feed
s12 T-100 feed
To add more streams to the above list.
Click here
OK

Figure 66. The Stream List Window

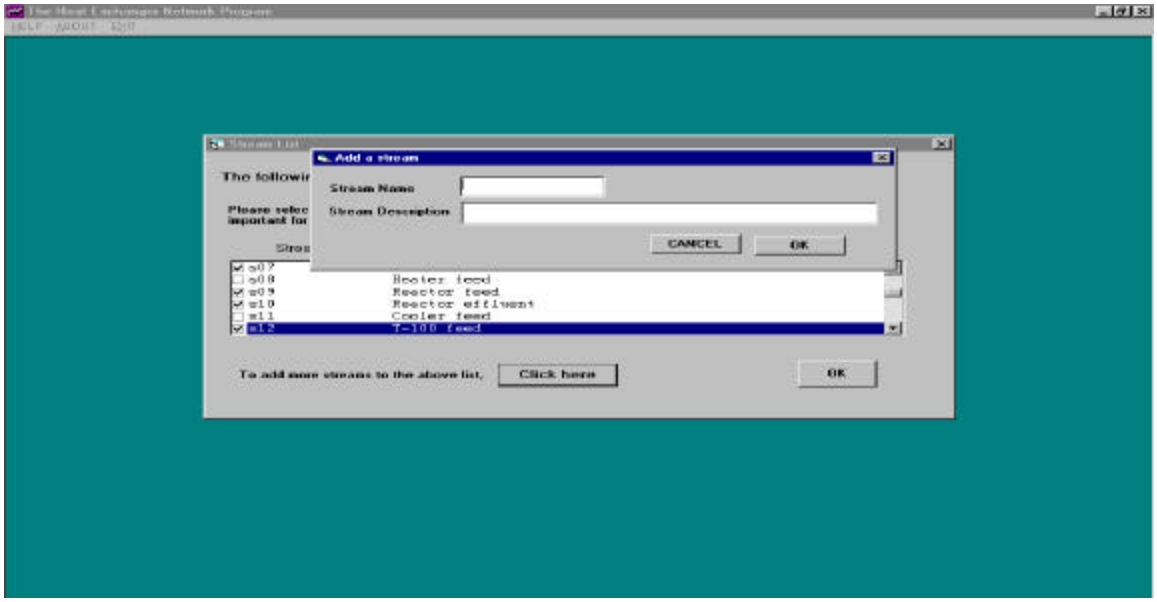


Figure 67 The Add Stream Window

Click on the 'Proceed' button on the welcome screen. The 'Stream List' window is now displayed on the screen. This is shown in Figure 66. The box in the center shows the list of all the process streams and their descriptions. This list has been automatically retrieved by the program from the information in the flowsheet diagram. Scroll up and down in the box to see the entire list. There is a check box available to the left of each stream name in the list. If a process stream is important for heat integration, the check box for that stream needs to be selected. For the aniline model, the following streams were determined to be important: s07, s09, s10, and s12. Select all of these streams in the list by clicking on their checkboxes.

The button 'Show the flowsheet diagram' at the top of the stream list window can be used to view the flowsheet diagram at any time. In addition to the streams listed, new streams can also be added. To add a stream, click the 'Click here' button at the bottom of the window. A small window shown in Figure 67 is displayed. A stream name and a description must be entered. Clicking the 'OK' button will add the stream to the list. For the aniline model, we do not want to add any streams. So, click the 'Cancel' button to go back to the 'Stream List' window.

Having selected all the important streams in the Stream List window, click the 'OK' button to continue. The next window displayed on the screen is the 'Retrieving Stream Data' window shown in Figure 68. A vertical line divides this window into two parts. The left side of the screen displays a list. This list contains all the streams, which were selected earlier in the 'Stream List' window. As can be seen from Figure 68, the four streams that were chosen as the important streams are present in the list.

The heat exchanger network program needs certain information for each stream in order to apply pinch analysis. This information includes temperature, flowrate, enthalpies and film heat transfer coefficient. The values of all of these variables have to be retrieved for each of the selected streams. The values for temperature and flowrate are automatically retrieved by the program from the results of economic optimization carried out earlier through the Advanced Process Analysis System. The values for enthalpies and film heat transfer coefficients have to be entered by the user. To understand how the data is retrieved, let us enter the data for the stream s07.

Click on the stream s07 in the list on the left side of the screen. On the right side of the screen, the stream name and stream description labels now show 's07' and 'Mixed stream' respectively. As can be seen in Figure 68, the temperatures and flowrate values for stream s07 have been automatically retrieved and displayed. The heat capacity and film coefficient values are initialized to the defaults, which are 0 and 100 respectively.

The enthalpy data for any stream can be entered as either constant heat capacity coefficients or temperature-dependent enthalpy coefficients. The variation in temperature is large for the streams in the aniline model. So, the temperature-dependent enthalpy coefficients are used for all the streams. To enter these coefficients for stream s07, select the 'Enthalpy coefficients' option. Once this option is selected, the button for modifying enthalpy data becomes enabled and a small frame for the average enthalpy coefficients of stream s07 can now be seen. This view is shown in Figure 69. The frame also shows the enthalpy formula used in the program.

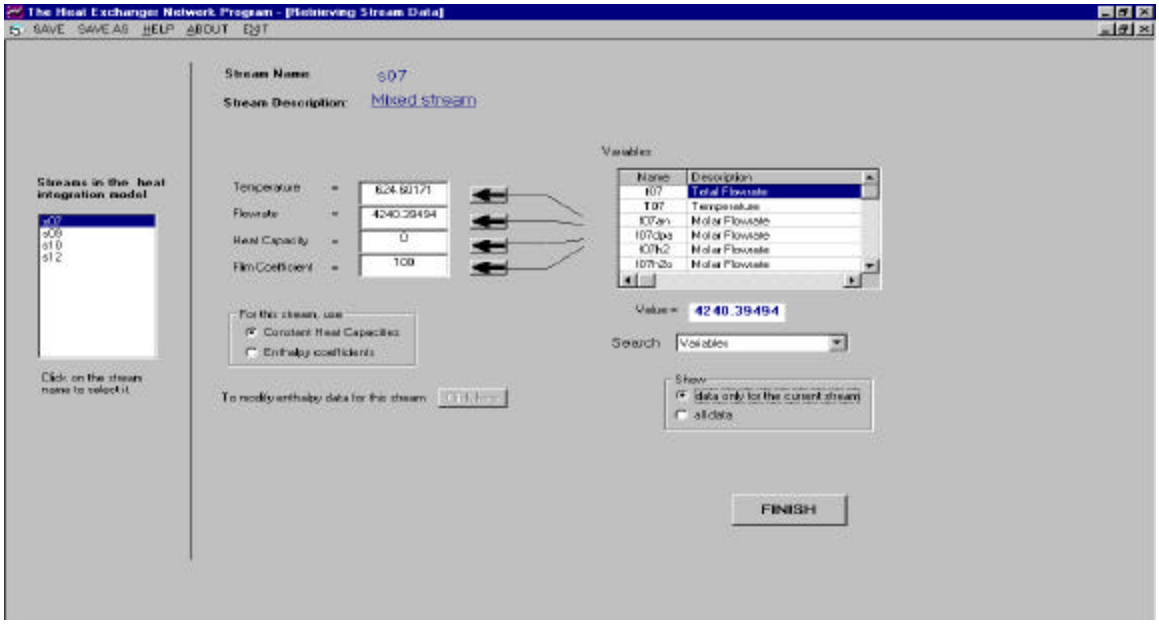


Figure68 . The Retrieving Stream Data Window

If the average enthalpy coefficient values are known for the stream, they can be entered in the corresponding boxes in the frame. Since, we do not know the average values, we will calculate them from the stream composition and the enthalpy coefficient values for the individual chemical species present in that stream. To perform these calculations, click the button for modifying the enthalpy data. When this button is clicked, the screen view changes to the 'Enthalpy Data' window shown in Figure 70.

The 'Enthalpy Data' window shows a list of all the chemical components present in the process. The components present in the reacting gases in aniline model are H_2, N_2, NH_3, H_2O, phenol, aniline and diphenylamine. These are automatically retrieved from FlowSim and displayed in the enthalpy data window. The table 'Components present in this stream' shows the components, which are present in stream s07. This table is empty as seen in Figure 70. This is because the components present in a stream need to be manually selected by the user and added to the table. From our knowledge about the process, we know that stream s07 has all seven of the above listed components. So, let us add all of these components to the table. Click on the component name in the list. The button with an arrow pointing towards the table now becomes enabled. Click on this button and the component gets transferred from the list to the table. After repeating this for all seven components, the screen looks as shown in Figure 71. The table 'Components present in this stream' now has seven components, but the list is not empty because there are components that are in different phases in the aniline process.

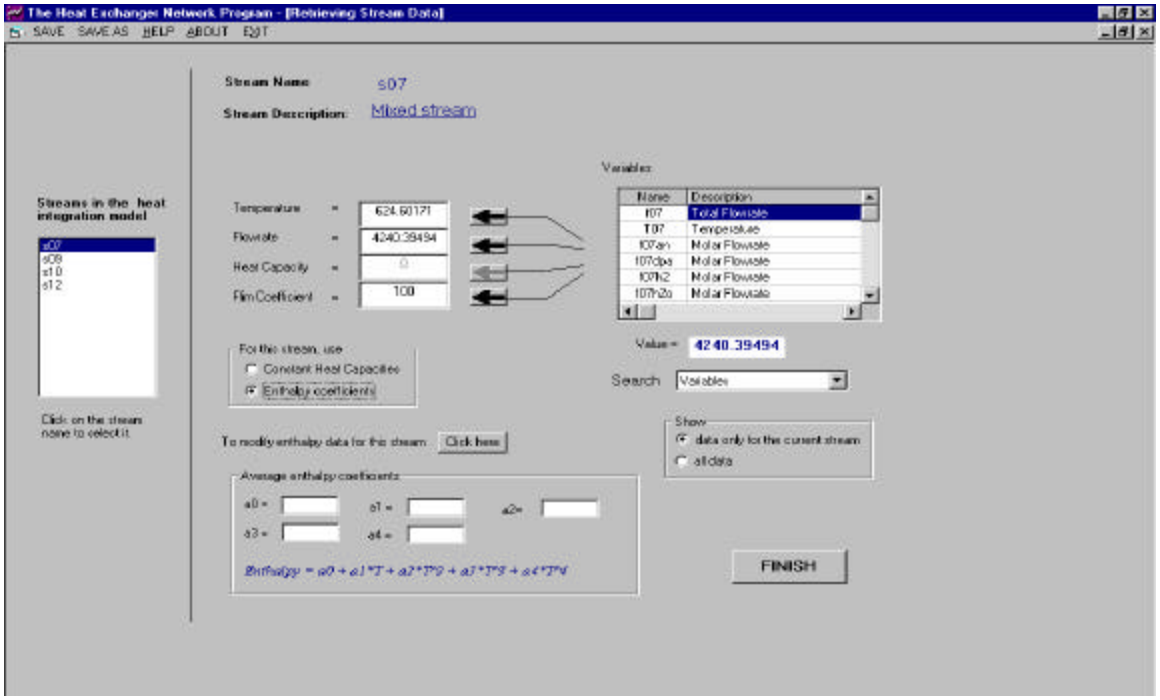


Figure 69. The Retrieving Stream Data Window with the Average Enthalpy Coefficients

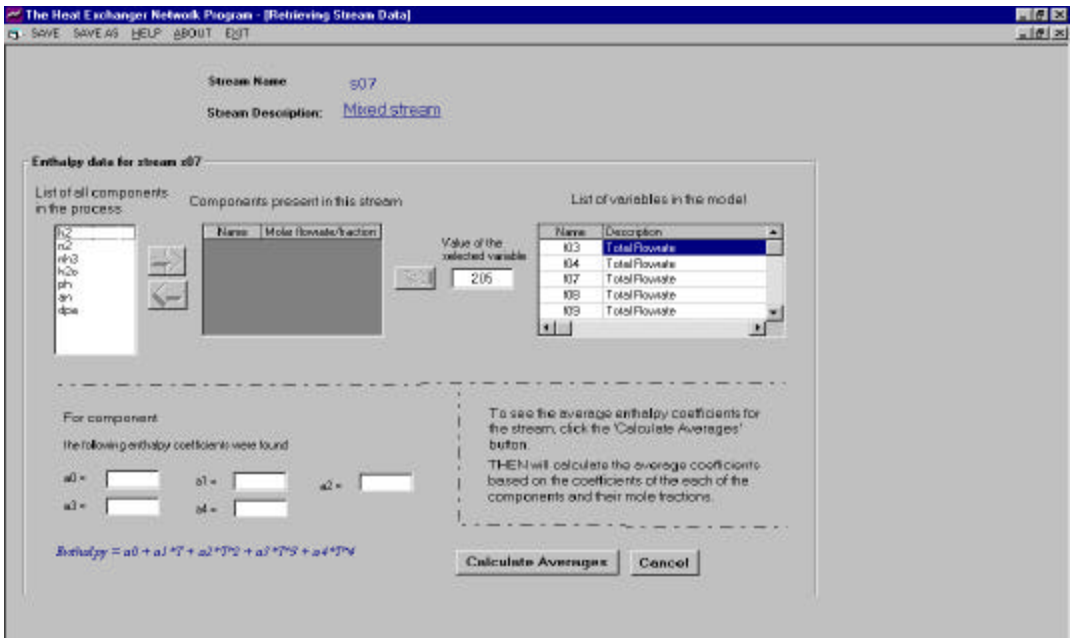

The Heat Exchanger Network Program - [Retrieving Stream Data]
SAVE SAVE AS HELP ABOUT EXIT
Stream Name s07
Stream Description: Mixed stream
Enthalpy data for stream s07
List of all components in the process
Components present in this stream
List of variables in the model
Value of the selected variable
For component
the following enthalpy coefficients were found
a0 =
a1 =
a2 =
a3 =
a4 =
To see the average enthalpy coefficients for the stream, click the 'Calculate Averages' button.
THEN will calculate the average coefficients based on the coefficients of the each of the components and their mole fractions.
Calculate Averages
Cancel

Figure 70. The Enthalpy Data Window

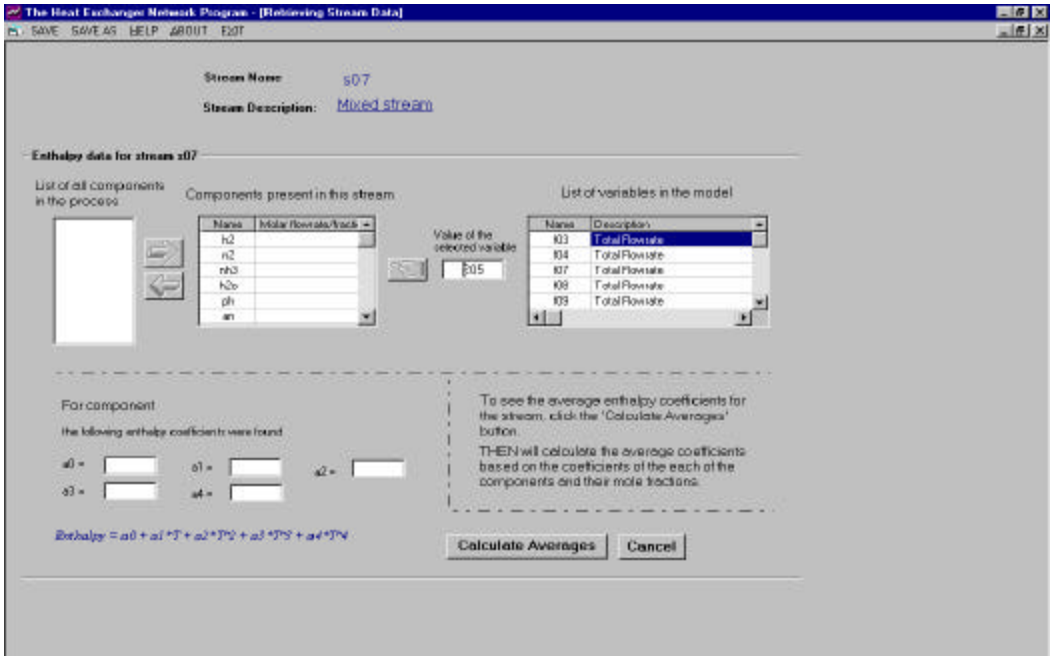

The Heat Exchanger Network Program - [Retrieving Stream Data]
SAVE SAVE AS HELP ABOUT EXIT
Stream Name s07
Stream Description: Mixed stream
Enthalpy data for stream s07
List of all components in the process
Components present in this stream
List of variables in the model
Value of the selected variable
For component
the following enthalpy coefficients were found
a0 =
a1 =
a2 =
a3 =
a4 =
To see the average enthalpy coefficients for the stream, click the 'Calculate Averages' button.
THEN will calculate the average coefficients based on the coefficients of the each of the components and their mole fractions.
Calculate Averages
Cancel

Figure71. The Enthalpy Window-2

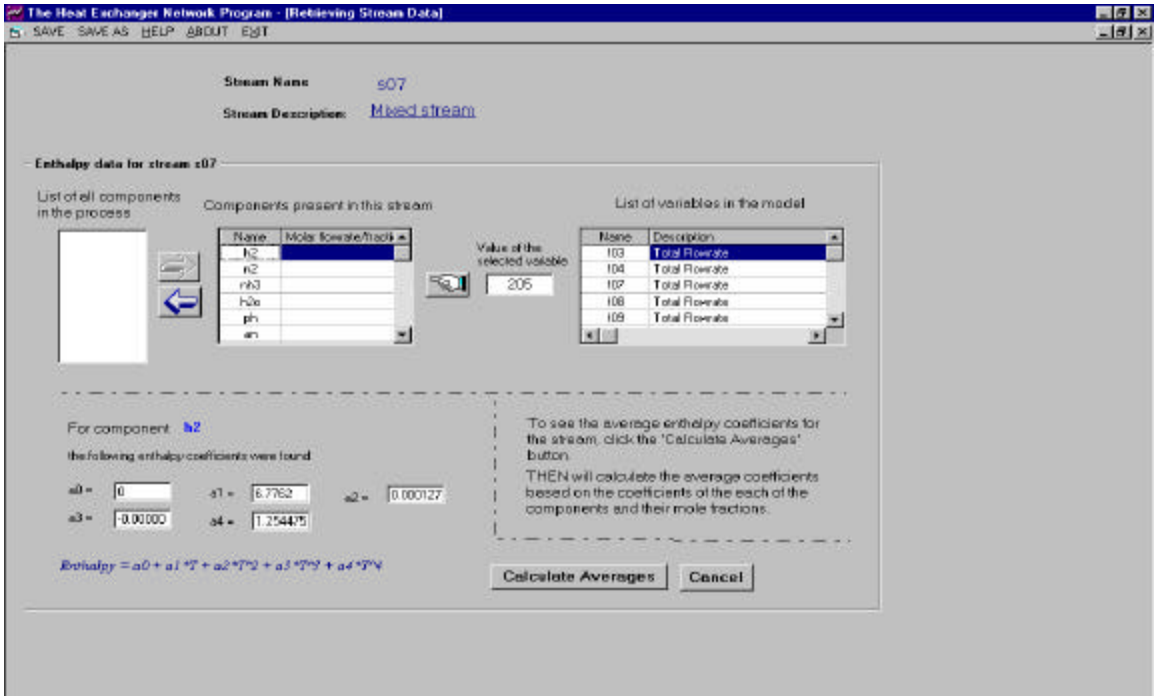

The Heat Exchanger Network Program - [Retrieving Stream Data]
SAVE SAVE AS HELP ABOUT EXIT
Stream Name s07
Stream Description Mixed stream
Enthalpy data for stream s07
List of all components in the process
Components present in this stream
List of variables in the model
Value of the selected variable
205
For component h2
the following enthalpy coefficients were found
a0 = 0
a1 = 6.7762
a2 = 0.000127
a3 = -0.00000
a4 = 1.254475
Enthalpy = a0 + a1 *T + a2 *T^2 + a3 *T^3 + a4 *T^4
To see the average enthalpy coefficients for the stream, click the 'Calculate Averages' button.
THEN will calculate the average coefficients based on the coefficients of the each of the components and their mole fractions.
Calculate Averages
Cancel

Figure 72 The Enthalpy Coefficients for H_2

To calculate the average enthalpy coefficients of the stream, the stream composition and the enthalpy coefficients of the individual chemical components are needed. The enthalpy coefficients of the chemical components were entered in the FlowSim program. These can be viewed in the Enthalpy window of Figure 71 by simply clicking on the component name in the table 'Components present in this stream'. For example, click on the first component H_2. The bottom part of the window now shows the enthalpy coefficients for H_2. This view is shown in Figure 72. Similarly, the enthalpy coefficients for all the other components can be viewed.

The second column of the table 'Components present in this stream' displays the molar flowrate or molar fraction of the component in the stream. As explained before, the average coefficients depend on the composition of the stream. The composition can be specified either in terms of molar flowrates of all the components or their molar fractions. These values have to be retrieved manually by the user. Let us retrieve the molar flowrates of the chemical components in stream s07.

The values we want to use for molar flowrates are from the results of on-line optimization. These values can be conveniently retrieved using the table 'List of variables in the model' on the right hand side of the widow. This window shows a list of all the variables (measured and unmeasured) with their descriptions. When a variable in this table is clicked, the value for that variable obtained as a result of economic optimization appears in the box titled 'Value of the selected variable'. The variable corresponding to molar flowrate of H_2 in stream s07 is f07h2. Search for this variable in the table. The measured variables in the model are listed first followed by the unmeasured variables, both in alphabetical order. When the variable f07h2 is clicked in the table, its value appears in the adjacent box. Now, click on the 'hand' button to take this value as the molar flowrate of H_2 in stream s07. The value is now copied into the table 'Components present in this stream' in the second column of the first row. Repeat this procedure for the seven components in stream s07. The screen now looks like Figure 73.

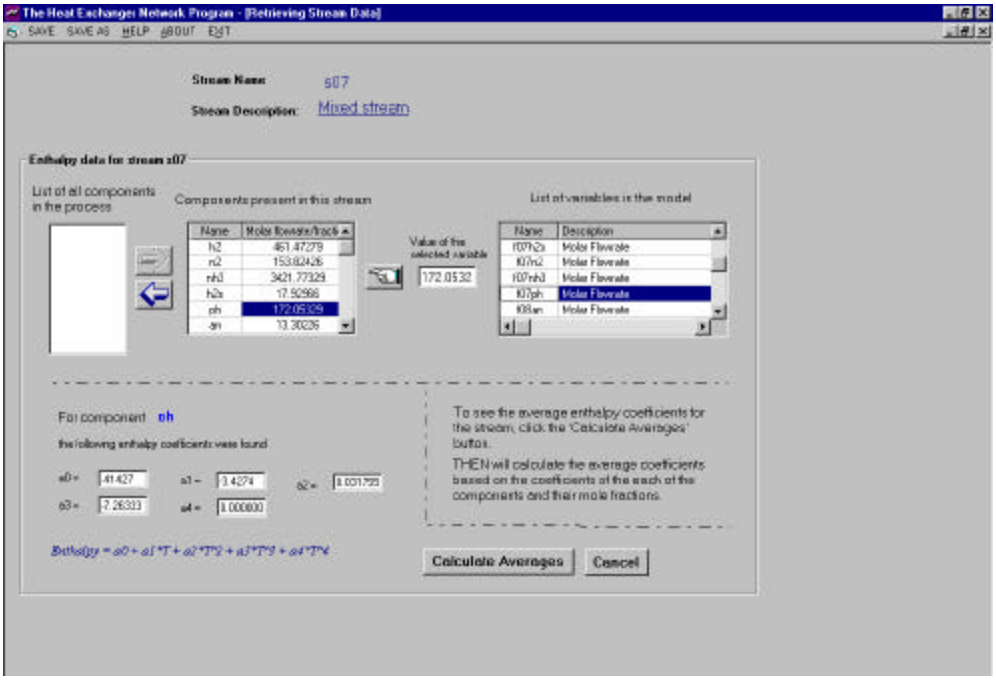

The Heat Exchanger Network Program - [Retrieving Stream Data]
SAVE SAVE AS HELP ABOUT EXIT
Stream Name s07
Stream Description: Mixed stream
Enthalpy data for stream s07
List of all components in the process
Components present in this stream
List of variables in the model
Name Molar flowrate/fract
h2 461.47279
n2 153.82426
nh3 3421.77329
h2o 17.92986
ph 172.05329
an 13.30236
Value of the selected variable
172.0532
Name Description
f07h2o Molar Flowrate
f07n2 Molar Flowrate
f07nh3 Molar Flowrate
f07ph Molar Flowrate
f08an Molar Flowrate
For component ph
the following enthalpy coefficients were found
a0 = 41.427
a1 = 3.4274
a2 = 3.031795
a3 = 7.26333
a4 = 1.000000
Enthalpy = a0 + a1*T + a2*T^2 + a3*T^3 + a4*T^4
To see the average enthalpy coefficients for the stream, click the 'Calculate Averages' button.
THEN will calculate the average coefficients based on the coefficients of the each of the components and their mole fractions.
Calculate Averages
Cancel

Figure 73. The Molar Flowrates in Stream S07

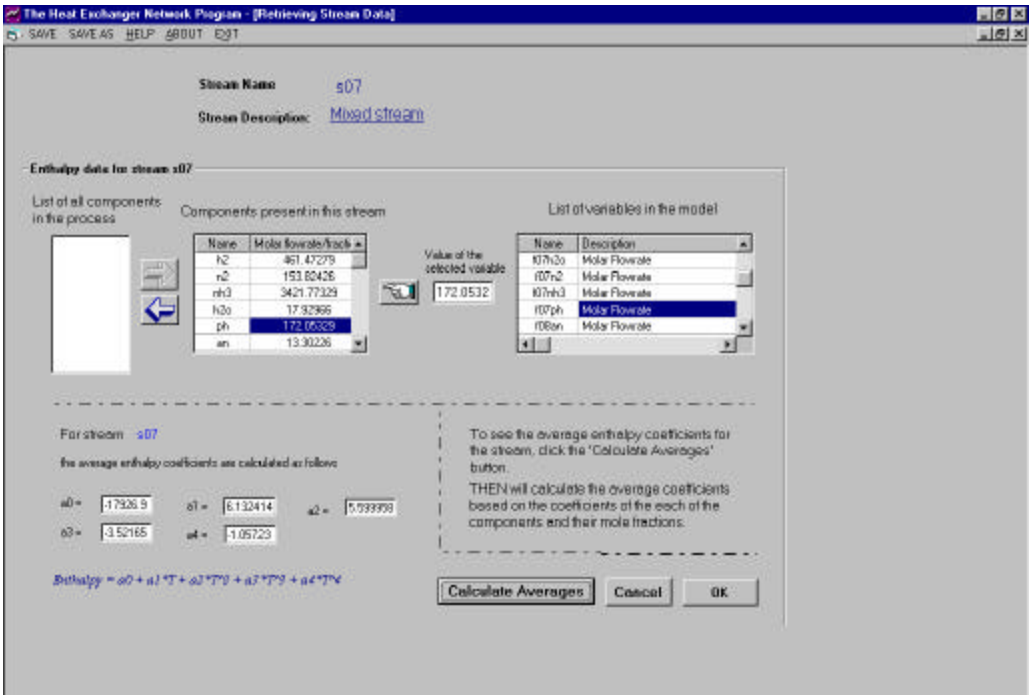

The Heat Exchanger Network Program - [Retrieving Stream Data]
SAVE SAVE AS HELP ABOUT EXIT
Stream Name s07
Stream Description: Mixed stream
Enthalpy data for stream s07
List of all components in the process
Components present in this stream
List of variables in the model
Name Molar flowrate/fract
h2 461.47279
n2 153.82426
nh3 3421.77329
h2o 17.92986
ph 172.05329
an 13.30236
Value of the selected variable
172.0532
Name Description
f07h2o Molar Flowrate
f07n2 Molar Flowrate
f07nh3 Molar Flowrate
f07ph Molar Flowrate
f08an Molar Flowrate
For stream s07
the average enthalpy coefficients are calculated as follows
a0 = -17926.9
a1 = 6.132414
a2 = 5.039998
a3 = -3.52165
a4 = -1.05723
Enthalpy = a0 + a1*T + a2*T^2 + a3*T^3 + a4*T^4
To see the average enthalpy coefficients for the stream, click the 'Calculate Averages' button.
THEN will calculate the average coefficients based on the coefficients of the each of the components and their mole fractions.
Calculate Averages
Cancel
OK

Figure 74. The Average Enthalpy Coefficients of Stream S07

Now that we have the composition of stream s07 in terms of molar flowrates and the enthalpy coefficients of the individual components, the average enthalpy coefficients for the stream can be calculated. Click the 'Calculate Averages' button at the bottom of the window. The program now calculates the average enthalpy coefficients for stream s07 and displays them in the bottom left part of the screen. Also, the OK button at the bottom of the window now becomes visible. This view is shown in Figure 74.

If you want to accept the average coefficient values calculated by the program, click 'OK'. If the values do not appear to be in the expected range and are not acceptable, click the 'Cancel' button. For the stream s07, we will accept the calculated values and click the 'OK' button. The screen view now goes back to the 'Retrieving stream data' window shown in Figure 69. The fields for the average coefficients at the bottom of this window are now filled with the values calculated by the program. This view is shown in Figure 75.

Now, the temperature, flowrate and enthalpy coefficients data for stream s07 have been entered and can be seen in the Figure 75. The final piece of information is the film heat transfer coefficient value. For the aniline model, an average film coefficient value of 51.9 Btu/ft^2-F-hr is estimated for all the process streams by the on-line optimization program. Change the default value of 100 to 51.9 as the film coefficient for stream s07. This completes the data retrieval for stream s07.

This procedure should be repeated for all of the streams listed on left side of the screen. For each of the streams, the temperature and flowrate will be automatically retrieved. The enthalpy coefficients should be calculated as done for stream s07. The film heat transfer coefficient values for all the streams should be 51.9. The data retrieval part for the aniline model is now complete and the 'Finish' button at the bottom of the screen should now be clicked.

When the 'Finish' button is clicked, the 'Build Model' window appears on the screen. This is shown in Figure 76. In this 'Build Model' window, the final step of dividing process streams into pairs of hot and cold streams is performed. This classification of streams constitutes the THEN model. In a THEN model, a hot stream is a stream that needs to be cooled and a cold stream is a stream that needs to be heated.

The table on the left side of the screen shows the list of process streams selected earlier in the program for heat integration. It shows the stream names as well as the descriptions. The two pairs of lists on the right side of the screen display the hot and cold streams in the stream model. Let us build the stream model for the aniline process.

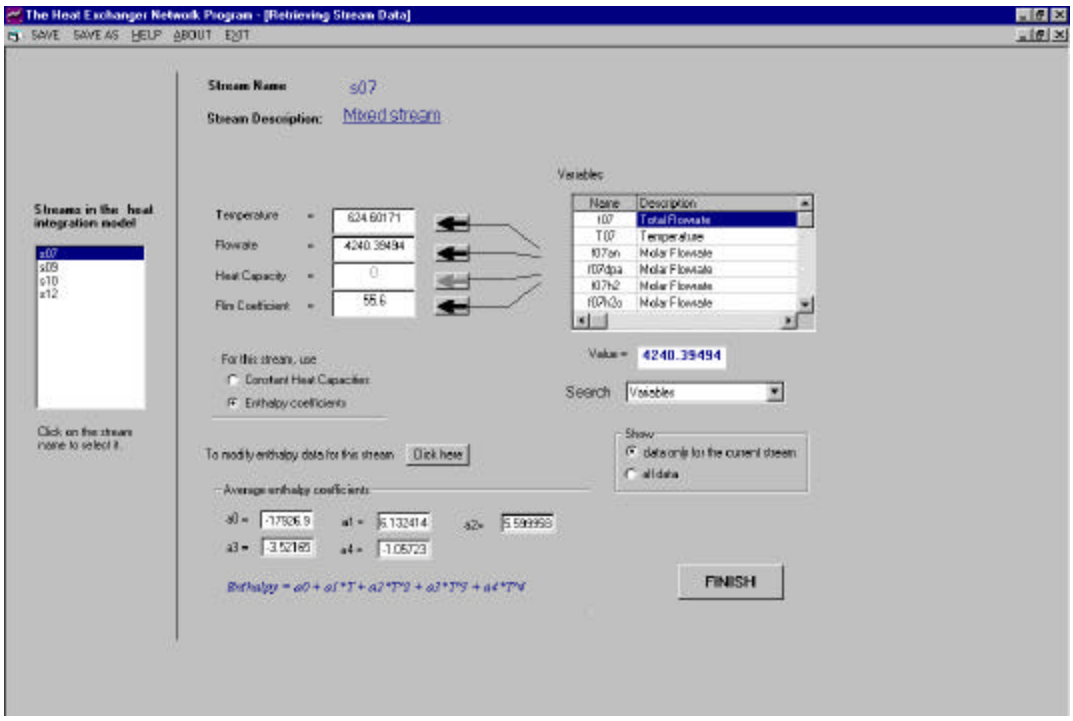


Figure 75. The Retrieving Stream Data Window-2

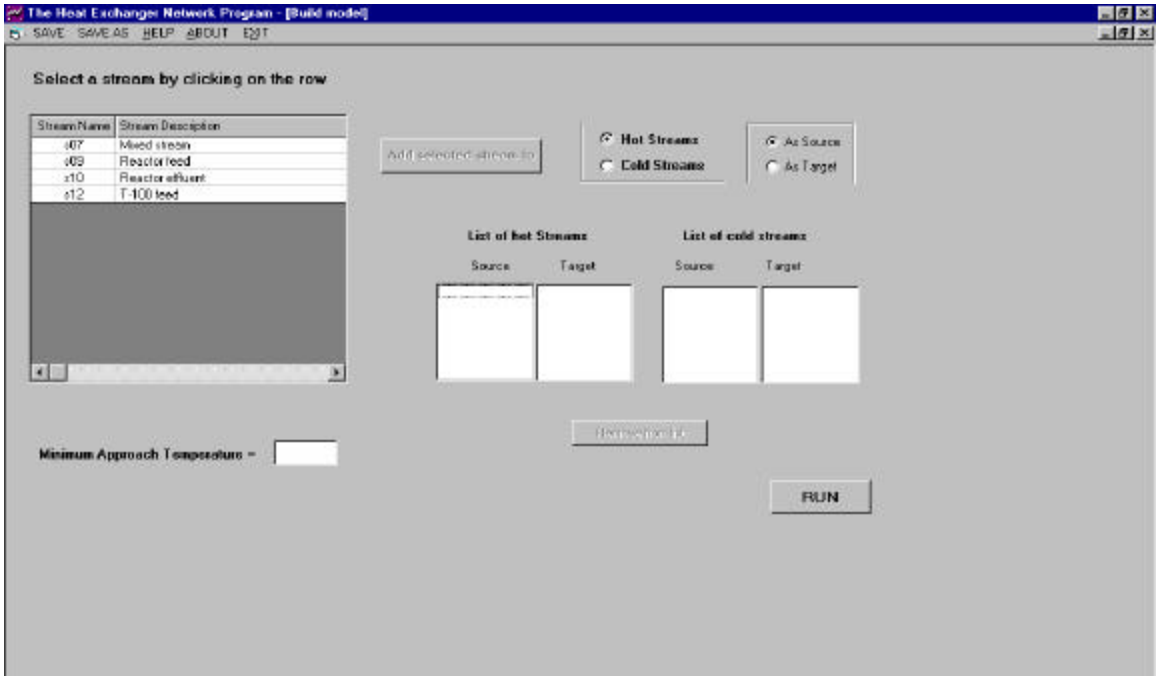


Figure 76. The Build Model Window

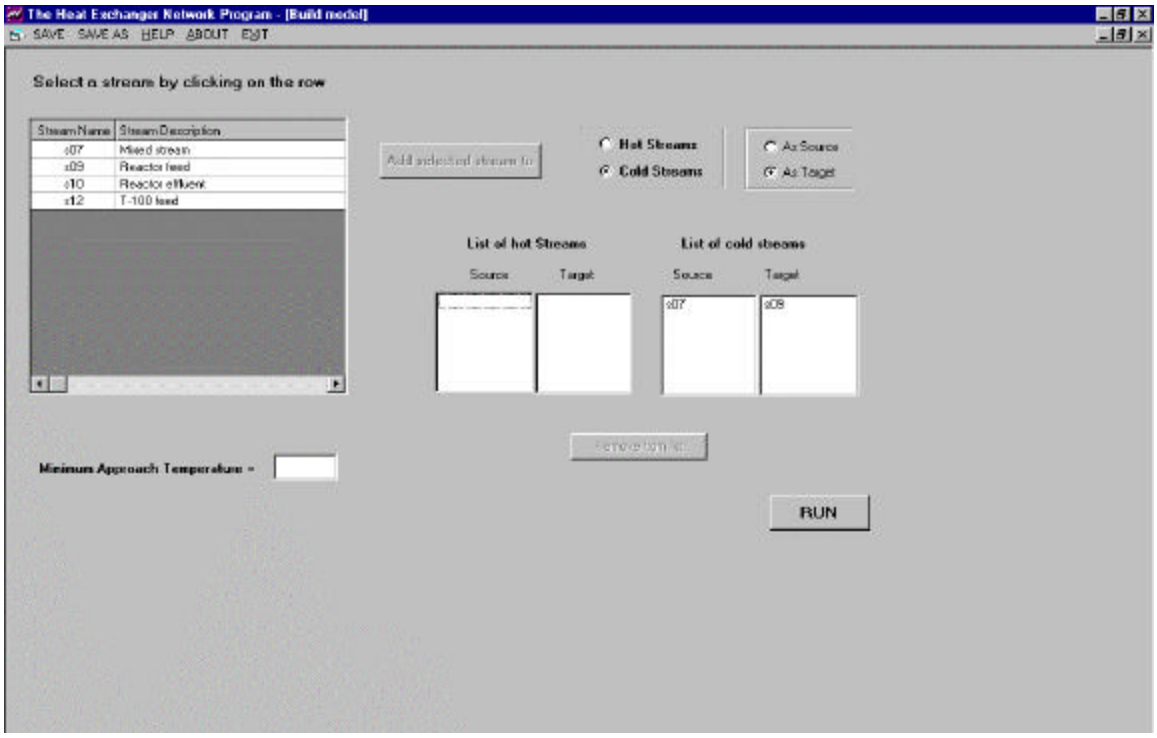


Figure77. The Build Model Window with one Cold Stream.

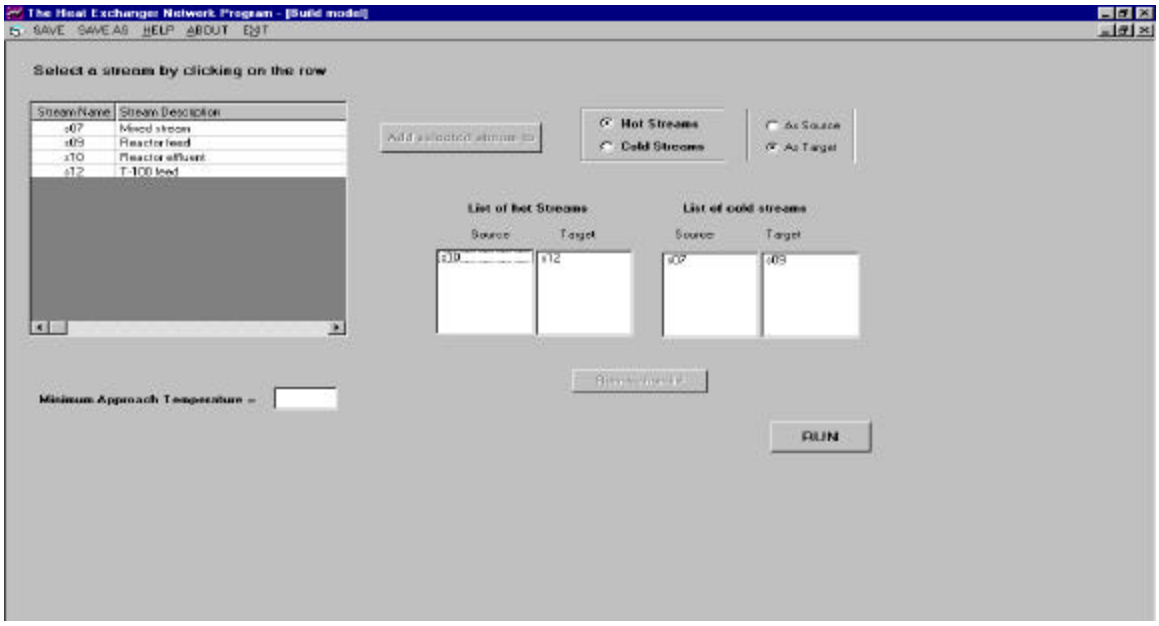


Figure 78. The Build Model with all the Hot an Cold Streams

From our knowledge of the aniline process, we know that stream s07 enters the cross heat exchanger and that stream s09 is the outlet stream from the heater. Therefore, streams s07 and s09 are the source and target of a cold stream respectively. To enter this cold stream, first select the stream s07 in the table. The button 'Add selected stream to' now becomes enabled. Select the 'Cold Streams' option and the 'As source' option. Now click the 'Add selected stream to' button. The stream s07 gets added to the list of cold streams as the source. Now click on the stream s09 in the table. Keep the 'Cold Streams' option and select the 'As target' option this time. Now, s07 and s09 are both added to the cold streams list as source and target respectivey. These two constitute one cold stream. The screen view now is shown in Figure 77.

Repeat this procedure for all the other streams. The hot stream pair for the aniline process is s07-s09. The cold stream pair is s10-s12. In these pairs, the first stream is the source and the second stream is the target. Once, we have entered all of these streams, the THEN model for the aniline process is complete. The 'Build Model' window with all the hot and cold streams is shown in Figure 78. The last piece of information needed is the minimum approach temperature between the streams. There is no fixed recommended value for this. We will enter an approach tempearture of 75°F to ensure that there is sufficient driving force for heat exchange between the streams.

The input part of the program is now over. **TO BE ABLE TO RUN THE REST OF THE HEAT EXCHANGE PROGRAM, YOU MUST NOW SAVE THE INFORMATION ENTERED SO FAR**. So, save the information entered by clicking the 'Save' button. The program displays the 'Save As' window shown in Figure 79. Save the model as 'aniline.hen' in the 'Examples' subdirectory of the program folder.

Now, click the 'Run' button on the 'Build Model' window. The program uses all of the information entered above and appiles concepts of pinch analysis to the aniline process. The next window that appears on the screen is the 'Output Window' shown in Figure 80.

Clicking the first button 'View and Save the GCC' on the 'Output Window' displays the 'Grand Composite Curve' on the screen. This is shown in Figure 81. It is a plot of enthalpy flows in the system versus temperature. The units for temperature and enthalpy are the same as for the input data entered. The temperatures are in Rankine and enthalpies are in Btu/hr. As seen in Figure 81, the curve touches the temperature-axis at one point. Since the process extends above and below this point, it needs a cold external utility and a hot external utility. The amount of cold utility is the enthalpy coordinate of the lowest point of the curve. This is about 4.1 MMBtu/hr as seen in the diagram. The amount of hot utility is the enthalpy coordinate of the highest point of the curve. This is about 3.1 MMBtu/hr as seen in the diagram. The exact amount of the cold and hot utilities can be seen in the output file, which is explained later.

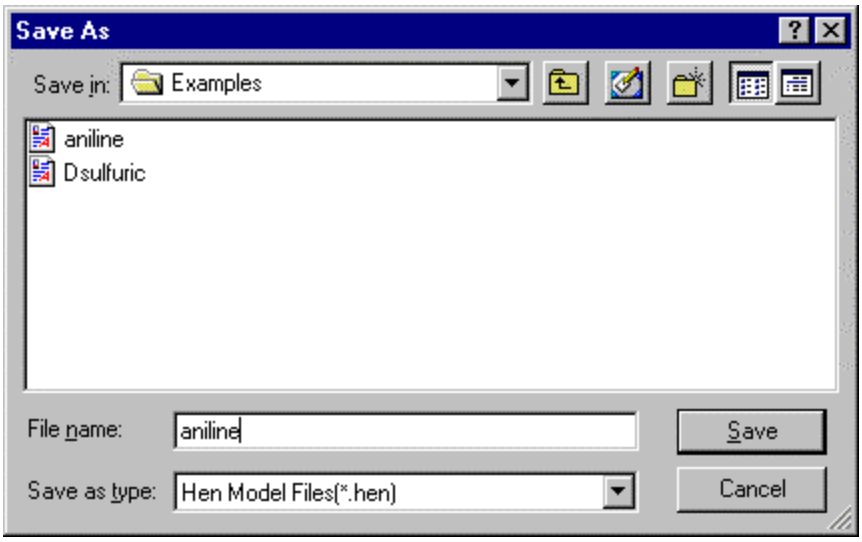


Figure 79. The Save As Window

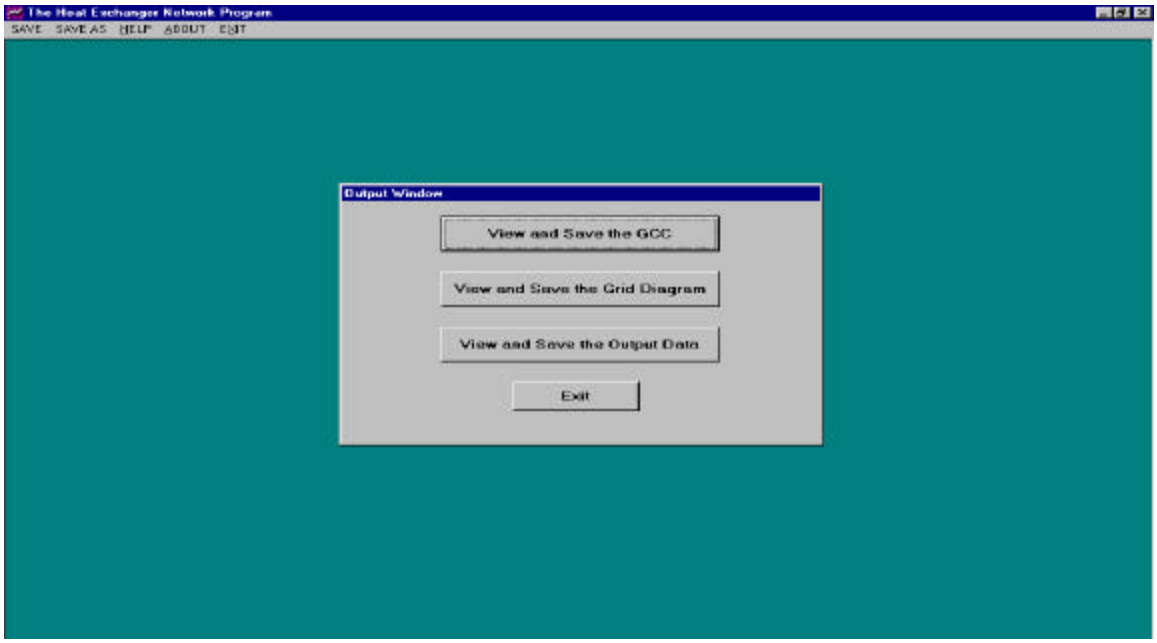

The Heat Exchanger Network Program
SAVE SAVE AS HELP ABOUT EXIT
Output Window
View and Save the GCC
View and Save the Grid Diagram
View and Save the Output Data
Exit

Figure 80. The Output Window

The menu bar at the top of the diagram provides options for viewing and printing the diagram. Clicking the 'View' button displays the commands to turn off the grid and show the data points. The 'Print Options' button can be used to set the number of copies and change the printer orientation. Clicking the 'Print' button will print the diagram to the default system printer. Click the 'Save' button to save the diagram in a 'Windows Metafile' format. The 'Help' button will display a brief description about the Grand Composite Curve. Closing the window brings the user back to the 'Output Window'. The second button 'View and Save the Grid Diagram' on the 'Output Window' displays the 'Network Grid Diagram'. This is shown in Figure 82. It is a graphical representation of the network solution designed by the program. It shows the arrangement of heat exchangers, heaters and coolers in the system. Red lines going from left to right represent hot streams and blue lines going from right to left represent cold streams. A red circle on a blue line means a heater and a blue circle on a red line is a cooler. Green circles joined by a vertical green line represent a heat exchanger between the streams on which the two circles lie.

The network grid diagram offers a very convenient way of understanding the solution network. Clicking on a unit in the diagram displays a small box, which shows all the necessary information for that unit. For example, clicking on a green circle will display the relevant information for the heat exchanger that it represents. This information includes the names of the hot and cold streams flowing through it, the heat load of the exchanger and the area of the exchanger. Clicking on a heater or a cooler will show the name of the stream flowing through it and its heat load. Similarly, clicking on a horizontal line will display the temperature, mass flowrate and average heat capacity of that stream. In Figure 85, the heat exchanger with index 1 has been selected by clicking, and the box at the bottom right side is showing the information for that heat exchanger.

Information about the grid diagram can be obtained as online help by clicking the 'Help' button in the menu bar at the top of the diagram. Other buttons in the menu bar are to set the view and print options. The 'Zoom' button allows the user to change the zoom of the diagram. The 'View' button can be used to display the printer lines. The 'Print' button will open the printer dialog box and print the diagram to the selected printer. Closing the window will take the user back to the 'Output Window'.

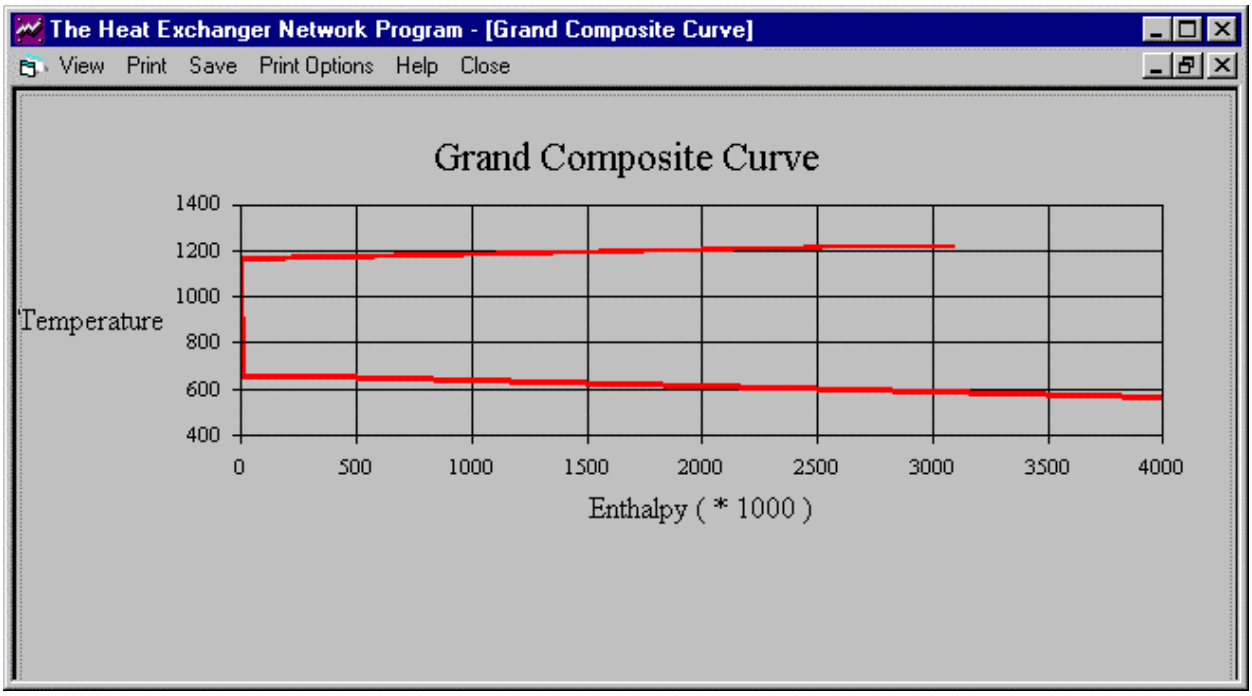


Figure 81.The Grand Composite Curve

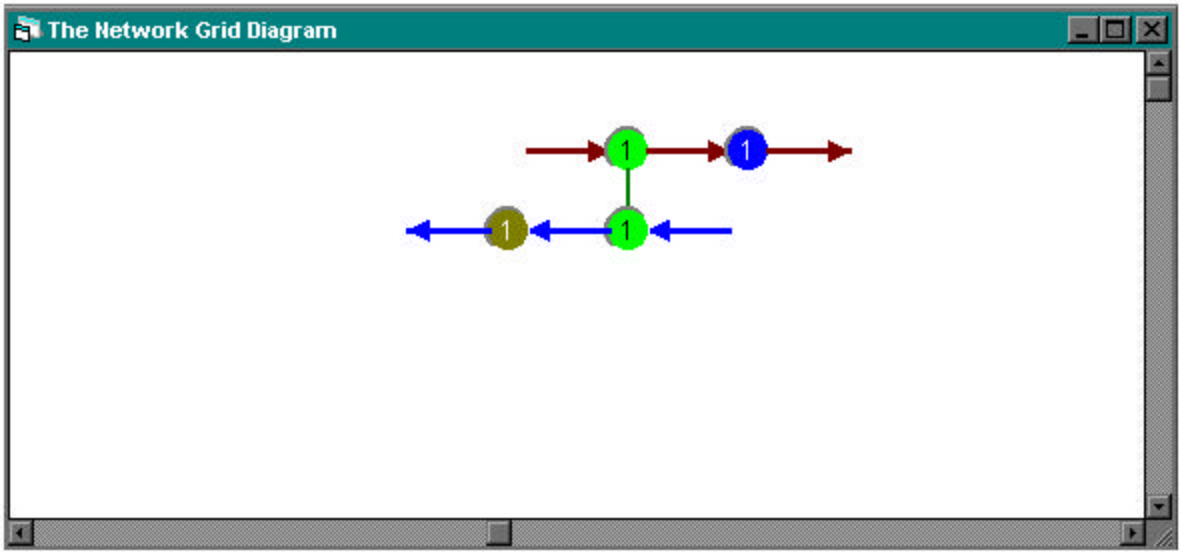


Figure 82. The Network Grid Diagram

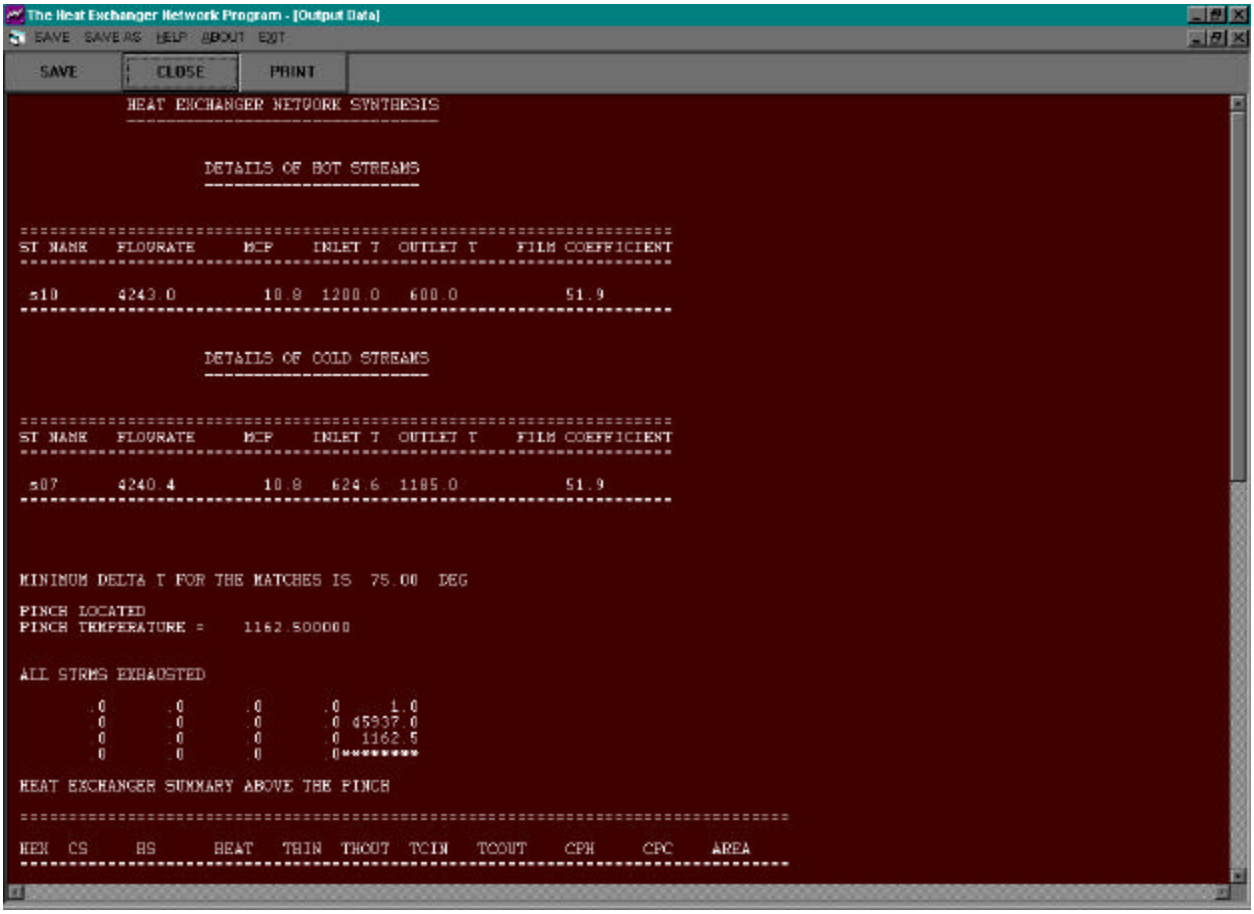

The Heat Exchanger Network Program - [Output Data]
SAVE SAVE AS HELP ABOUT EXIT
SAVE
CLOSE
PRINT
HEAT EXCHANGER NETWORK SYNTHESIS
DETAILS OF HOT STREAMS
ST NAME FLOWRATE MCP INLET T OUTLET T FILM COEFFICIENT
s10 4243.0 10.0 1200.0 600.0 51.9
DETAILS OF COLD STREAMS
ST NAME FLOWRATE MCP INLET T OUTLET T FILM COEFFICIENT
s07 4240.4 10.0 624.6 1185.0 51.9
MINIMUM DELTA T FOR THE MATCHES IS 75.00 DEG
PINCH LOCATED
PINCH TEMPERATURE = 1162.500000
ALL STRMS EXHAUSTED
.0 .0 .0 .0 1.0
.0 .0 .0 .0 45937.0
.0 .0 .0 .0 1162.5
.0 .0 .0 .0********
HEAT EXCHANGER SUMMARY ABOVE THE PINCH
HEN CS HS HEAT THIN THOUT TCIN TCOUT CPH CPC AREA

Figure 83. The Output Data Window

The third button in the output window, the ‘View and Save the Output Data’ button shows the output text file in a window as shown in Figure 83. Using horizontal and vertical scroll bars, the user can see the entire output text. The 'Print' button at the top of the window prints output file to the default printer. On clicking the ‘Save’ button, the program opens the 'Save As' window and requests the user to specify the filename. Let us save the output as file 'out.dat' in the Examples subdirectory of the program folder. Click the 'Close' button to go back to the Output Menu window.

The execution of the THEN program is complete. The results have been displayed in the grand composite curve, network grid diagram and the output data file forms. Let us look at the results more closely and interpret the solution generated by THEN.

Using the Results from THEN

The Grand Composite Curve (GCC):

The GCC for the aniline process is shown in Figure 81. It is a plot of temperature on the Y-axis versus the enthalpy flow on the X-axis. If the curve touches the temperature-axis except at its endpoints, it is a pinched process, and the temperature corresponding to that point is the pinch temperature. If the curve touches the X-axis at its uppermost point, the process is ‘below

the pinch' process. If it touches at the lowermost point, it is an 'above the pinch' process. In Figure 81, the GCC does not meet the temperature axis at one of its endpoints. Hence, it is a pinched process.

Also, the GCC can be used to determine the minimum amount of hot and cold utilities needed by the process. To find the amount of hot utility required locate the topmost point of the curve and read its X-coordinate which is equal to the amount of hot utility. Similarly, to get the amount of cold utility required, locate the bottommost point of the curve and read its X-coordinate. For the aniline process, from Figure 81, it can be seen that the amount of hot utility is about 3.1 MMBtu/hr and the amount of cold utility is about 4.1 MMBtu/hr.

The Network Grid Diagram:

The network grid diagram for the aniline process is shown in Figure 82. Let us examine this diagram to understand the new heat exchanger network structure for this process. The horizontal red line at the top running from left to right represent the hot stream s10. The horizontal blue line at the bottom running from right to left represents the cold stream s07. The blue circle (numbered 1) on stream H1 indicates that this stream requires a cooler. The red circle (numbered 1) on stream C1 indicates that this stream requires a heater. There is one pair of green circles (numbered 1) joined by vertical green lines. This represents the main heat exchanger in the process. The exchanger exchanges heat between the two streams on which the two circles lie. For example, heat exchanger 1 (the pair of green circles with number 1) is exchanging heat between hot stream s10 and cold stream s07. Thus, it can been seen from the grid diagram that the aniline process needs one heat exchanger, one heater and one cooler in the new network solution.

The Output Data File:

Now, let us examine the output data generated by THEN. The complete output file for the above problem is given in Table 6. In Table 6, the first two sections 'Details of Hot Streams' and 'Details of Cold Streams' list a summary of the input information entered by the user. This consists of the data for hot and cold streams followed by the specified minimum approach temperature for the matches.

The input summary is followed by the results for the simple process. The first three lines of the output show that the given problem was a pinched problem.

This is followed by a matrix of values which is the solution array generated by THEN for the problem above and below the pinch. These values can help in understanding the matches made by the program to arrive at the solution. However, the most important part of the output is the Heat Exchangers, Heaters and Coolers summary tables, which follow on the next two pages.

The heater summary above the pinch shows that we need one heater in the system. The heating load for the heater on the stream s07 is 2.8 MMBtu/hr. Stream s07 enters the heater at 1125^{o}R and leaves at 1185^{o}R.

The heat exchanger summary below the pinch shows that there should be one heat exchanger between streams s07 and s10. For exchanger 1, the heat transfer rate will be 23.0 MMBtu/hr. Also, it gives the inlet and outlet temperatures for both the streams. Note that the area of the heat exchanger (11810.820 ft^2) has been calculated using the film heat transfer coefficient supplied in the data.

Next comes the cooler summary below the pinch. It shows that we need one cooler in the system. The cooling load for the cooler on the stream s10 is 4.6 MMBtu/hr. Stream s10 enters the cooler at 700.5^oR and leaves at 600^oR.

Next comes the information about the loops identified in the network. A loop is any path in the heat exchanger network that starts at some point and returns to the same point. For the aniline process, there are no loops in the network.

Finally, the last two lines of output give the minimum hot and cold utilities needed for this process. Thus, for the aniline process, 3044976 Btu/hr of heat needs to be added by use of an external hot utility. Similarly, 4903696 Btu/hr of heat needs to be removed by use of an external cold utility.

Note that just above the printout of the solution array is a message which says if all the streams were exhausted or not. If the message is 'all streams exhausted', THEN has successfully generated the heat exchanger network. If the message is 'Error- not all streams exhausted', THEN has failed to solve the problem. In this case, the order of the streams in the input data should be changed. For example, the data for stream s10 should be entered before stream s07. The program uses a solution method that is sensitive to the order in which the stream data is entered.

To summarize, the aniline process is a pinched process, and it needs one heat exchanger, one cooler, and one heater for maximum energy utilization. The minimum amount of hot utility is 3044976 Btu/hr and the minimum amount of cold utility is 4903696 Btu/hr.

This concludes the implementation of the Heat Exchanger Network program in the Advanced Process Analysis System. The next step of the Advanced Process Analysis System is calculation of pollution indices. Click on the 'Pollution Index' button in the Advanced Process Analysis Desk to call the pollution index program.

Table 6. THEN Solution for the Contact Process- Output Data File

```
                    DETAILS OF HOT STREAMS

ST NAME   FLOWRATE     MCP    INLET T  OUTLET T    FILM
                                                COEFFICIENT

  s10      4243.0      10.8   1200.0    600.0      51.9

                   DETAILS OF COLD STREAMS

ST NAME   FLOWRATE     MCP    INLET T  OUTLET T    FILM
                                                COEFFICIENT

  s07      4240.4      10.8   624.6     1185.0     51.9

MINIMUM DELTA T FOR THE MATCHES IS  75.00  DEG

PINCH LOCATED
PINCH TEMPERATURE =   1162.500000

ALL STRMS EXHAUSTED

        .0      .0      .0      .0     1.0
        .0      .0      .0      .0 45937.0
        .0      .0      .0      .0  1162.5
        .0      .0      .0      .0********

HEAT EXCHANGER SUMMARY ABOVE THE PINCH

HEX   CS   HS    HEAT    THIN    THOUT    TCIN    TCOUT
 CPH      CPC      AREA

HEATER SUMMARY ABOVE THE PINCH

HEATER  CNO    HEAT     TCIN    TCOUT     CPC

  1.0   1.0  2756222.0  1125.0  1185.0  45937.0

ALL STRMS EXHAUSTED

        .0      .0      .0      .0     1.0
        .0      .0      .0      .0 45937.0
        .0      .0      .0      .0   662.1
        .0      .0      .0      .0      .0
       1.0 45937.0   662.1      .0********
       1.0    82.5  1162.5 49505.3      .0
```

```
HEAT EXCHANGER SUMMARY BELOW PINCH

HEX   CS   HS    HEAT    THIN    THOUT    TCIN    TCOUT
 CPH       CPC       AREA

1.   s07  s10  .230E+08  1200.0  699.60   624.60  1125.0
.46E+05  .46E+05  11810.820

COOLER SUMMARY BELOW THE PINCH

COOLER  CNO    HEAT     THIN    THOUT     CPH

 1.0    1.0  4624910.0  700.5   600.0    46019.5

NO LOOPS PRESENT IN THIS NETWORK

THE MINIMUM HOT UTILITY REQUIREMENT IS:   3044976.000000

THE MINIMUM COLD UTILITY REQUIREMENT IS:  4903696.000000
```

VIII. USING THE POLLUTION INDEX PROGRAM

Upon clicking the 'Pollution Index' button in the Advanced Process Analysis Desk, the first window presented to the user is the 'Process' window shown in Figure 84.

The table 'Stream List' shows the list of all input and output streams in the process. This list is entered by the user. The first column of the table gives the stream name, the second column gives the total flowrate of the stream and the third column gives the type of the stream. As discussed in Section I, the streams important for pollution index calculations are the input and output streams, and the output streams are further divided into product and non-product streams.

To enter a stream into the list, click on the 'Add Stream to list' button. This will bring up a 'Please enter a stream name' prompt. Click OK. Enter the stream name and the stream type. This is shown in Figure 84. Click on the 'Add Stream to list' button again. At this point, the total flowrate column shows 0. To enter the total flowrate, choose the 'Mass/Mole Fractions of Components' radio button. The 'Load Data into Total Flow rate for stream' button will appear. Click on the 'Total Flowrate' variable in the Variables table. Then, click on the 'Load Data into Total Flow rate for stream' button to enter the value into the Total Flowrate window. This is shown in Figure 85. Click on the 'Update Stream Information' button to load the value into the stream list table.

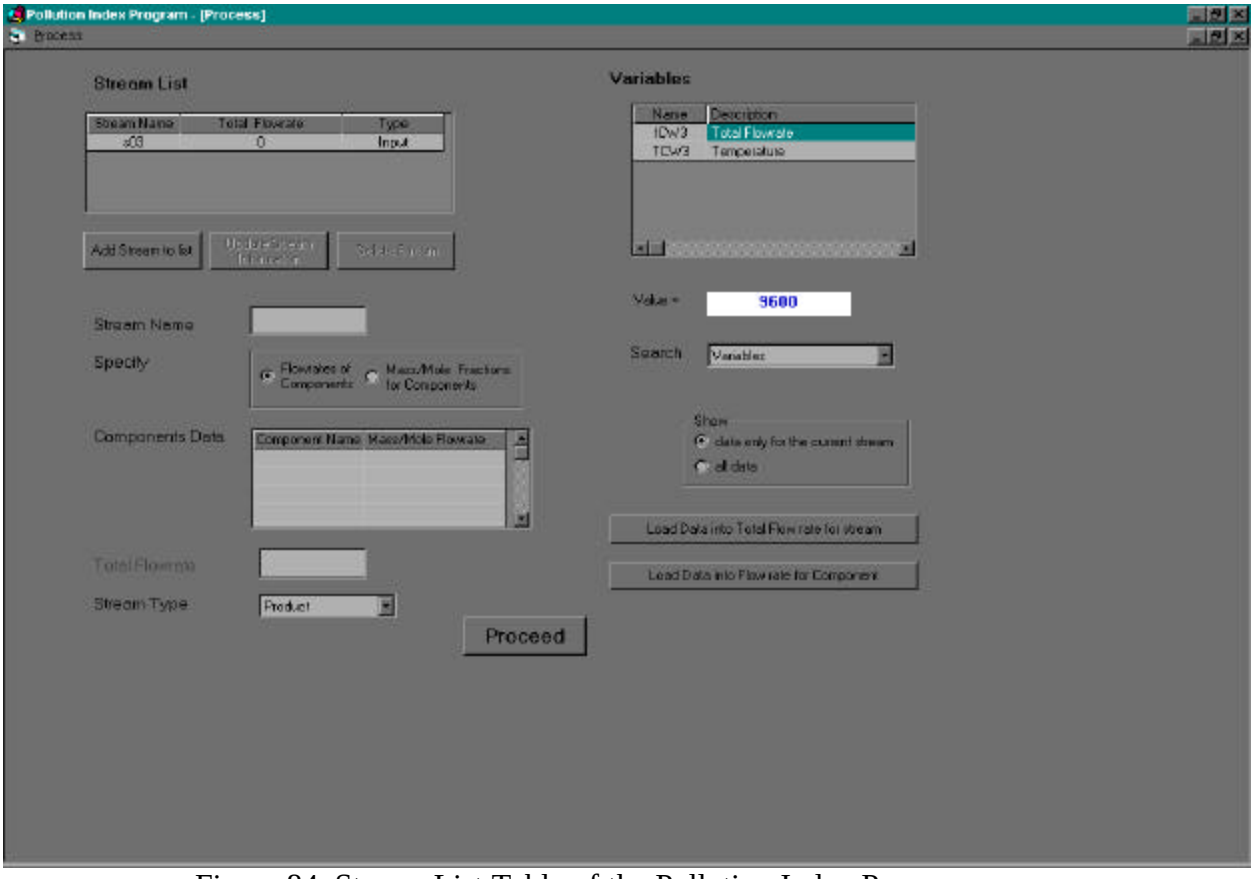


Figure 84. Stream List Table of the Pollution Index Program

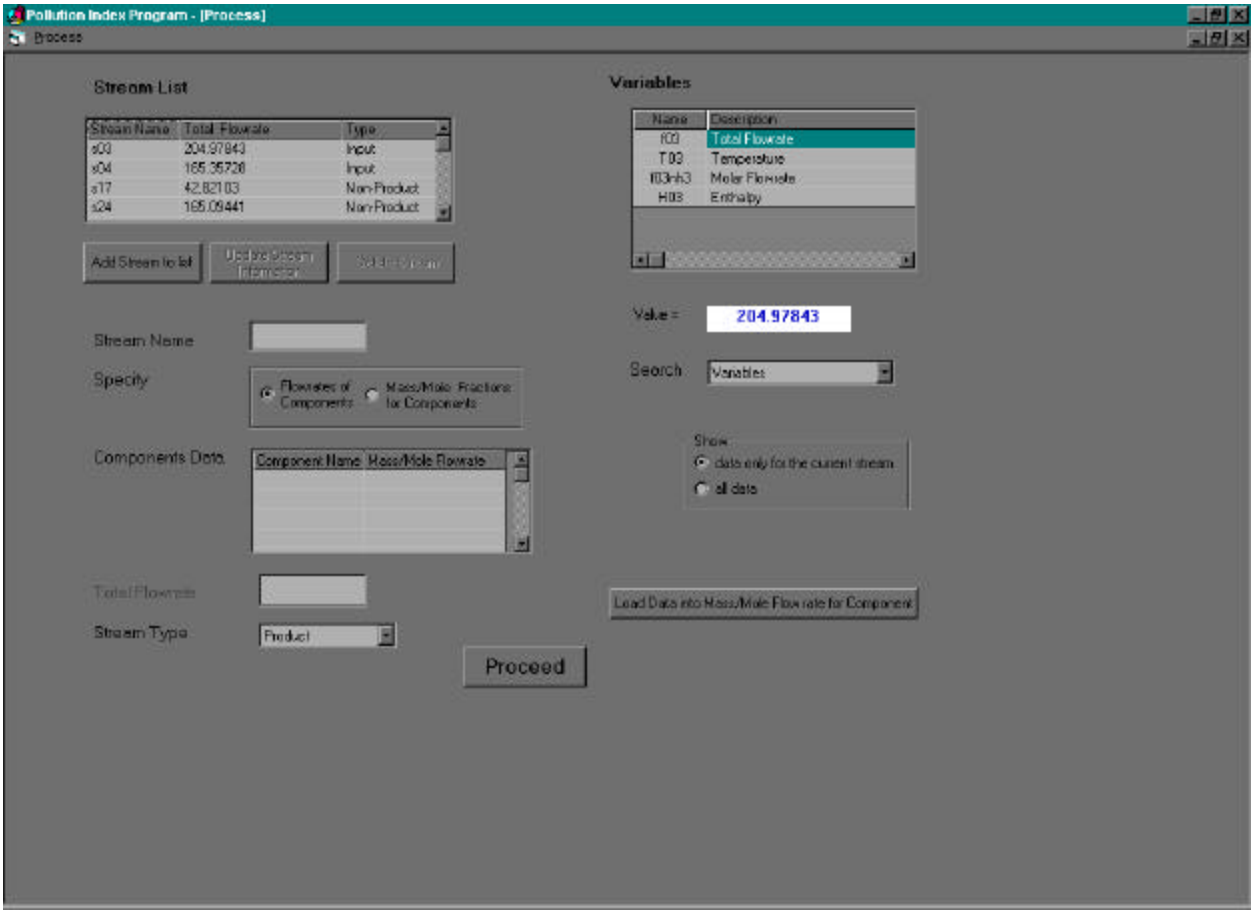


Figure 85 . The Process screen with Stream S03

Calculation of pollution indices requires the composition of the process streams. The composition can be specified either in terms of molar flowrates or mole fractions. These values can be conveniently retrieved from the results of on-line optimization. Let us retrieve the values for the first stream in the list, s03. Click on the stream, s03 in the table 'Stream List' in Figure 88. Choose the radio button with the option 'Flowrates of Components' to specify the composition. Now, let us retrieve the flowrates of the individual components in stream s03 as described below.

In Figure 85, the table 'Variables' on the right-hand side at the top shows the names and descriptions of all the measured and unmeasured variables in the aniline process model. Select the radio button for the option 'data only for the current stream'. When this option is selected, the table 'Variables' only shows the variables that are associated with that stream. The screen view now is shown in Figure 85. The variables associated with stream s03 can be seen in the table 'Variables' in Figure 85. Stream s03 is the ammonia feed stream, and it contains only ammonia. In the 'Variables' table, f03nh3 is the molar flowrate of ammonia in stream s03. Let us enter these values in the 'Components Data' table as described below.

In the 'Component Data' table, enter NH3 in the first row of the component name column. Now click on the variable f03nh3 in the 'Variables' table. The value field below the 'Variables' table now shows the value of f03nh3 obtained as a result of economic optimization. To take this value as the molar flowrate of NH3, click the button 'Load Data into Mass/Mole Flowrate for Component'. The components of the stream s03 have been entered and the

composition of stream s03 is now completely specified. The stream type of stream s03 is 'input' as entered by the user. The screen view now is shown in Figure 86. The above changes made to the composition data for stream s03 need to be updated. Click on the 'Update Stream Information' button to save the changes.

Repeat the same procedure for all the other streams in the 'Stream List' table. Click on each stream in the table. Enter the component names and retrieve their flowrates from the 'Variables' table. If you do not see the required variable in the table, choose the 'all data' option. For the output streams, change the default type from 'product' to 'non-product' wherever necessary. In the aniline process, the stream s17, the gaseous purge, and the stream s24, the water product, and the streams CW2, CW4, CW6 and CW8, the cooling water products, are the non-product streams. For each stream, after the changes are done, click the 'Update Stream Information' button.

When the composition information for all the streams in the 'Stream List' table has been entered, click the 'Proceed' button. The 'Components' window is now displayed on the screen. This is shown in Figure 87. This window is used to enter the specific environmental impact potentials of the various components in the process. As discussed in Section I, there are nine categories of environmental impacts. The specific environmental impact potential values have to be entered for each component for each of the nine types of impact.

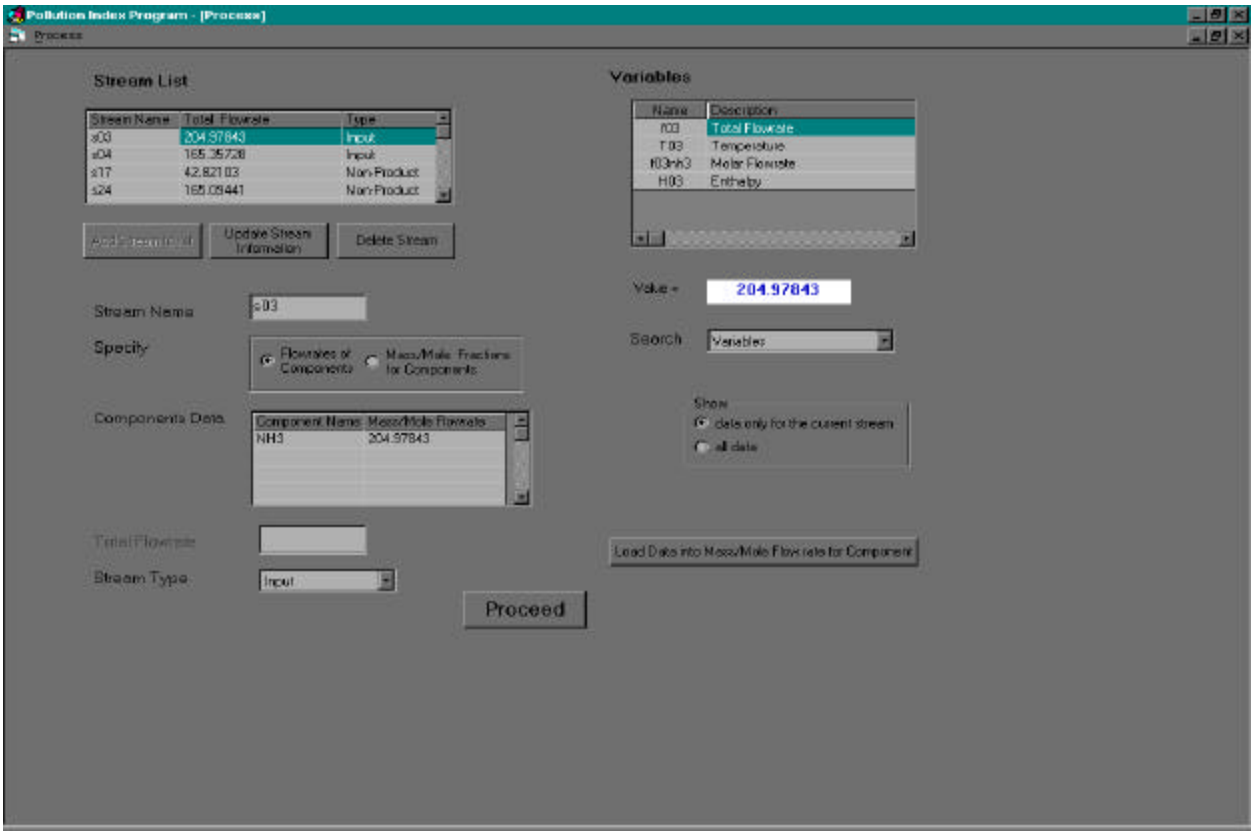


Figure 86. The Composition Data for Stream S03

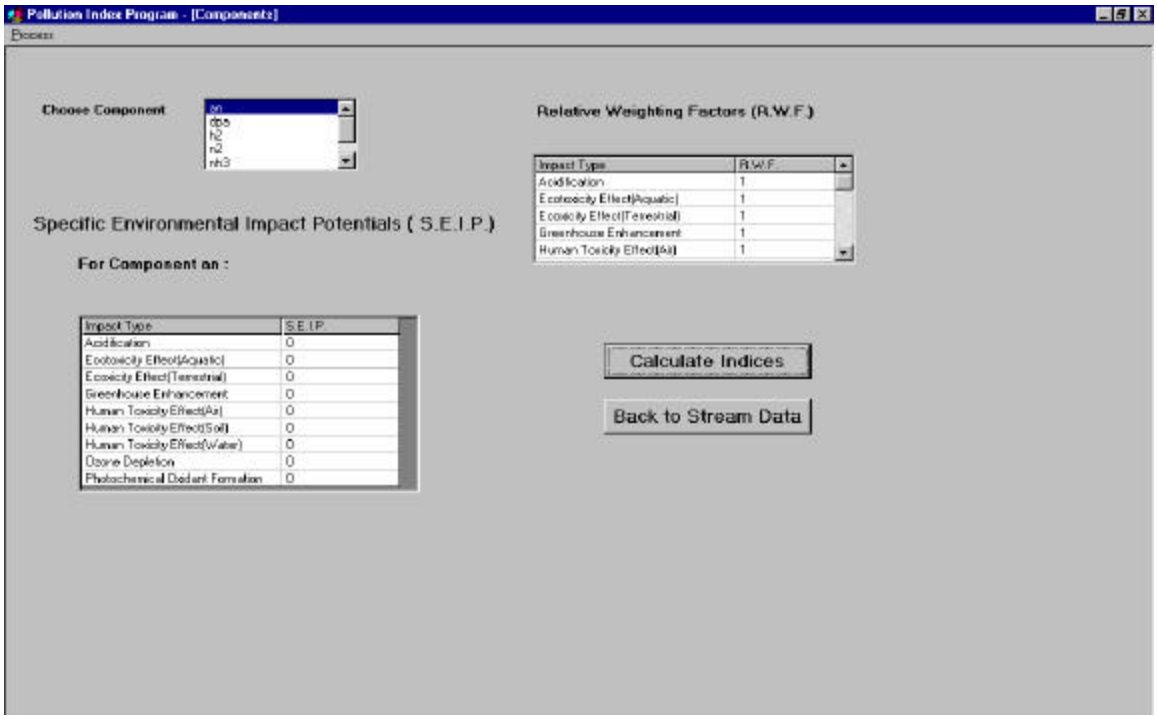


Figure 87 The Components Window

The 'Choose Component' table gives a list of all the components present in the input and output streams of the model. The impact potentials values for the components of the aniline process were obtained from the report on environmental life cycle assessment of products (Heijungs, 1992) published by the EPA. The chemicals with non-zero environmental impact potentials (aniline, phenol, ammonia and diphenylamine) for the aniline process are shown in Table 7. H_2, N_2 and H_2O have zero environmental impact potentials for all categories.

Since the default values of all impact potentials in the program are zero, the values for NH_3, phenol, aniline and diphenylamine need to be changed. Scroll down in the component list and select NH_3. Now click on the S.E.I.P. (specific environmental impact potentials) column in the first row. This row is for the impact type 'acidification'. Enter the value 1.833153. Continue for each impact that has a non-zero value as shown in Table 7. Repeat this for the remaining chemicals with impact potentials. The final piece of information needed is the relative weighting factors. For the aniline process, let us keep the default values of 1 for all the weighting factors. All of the information necessary for the calculation of the pollution indices has been entered in the program. Now, click on the 'Calculate Indices' button to view the values of the six pollution indices defined earlier in Section I.

Table 7. Environmental Impact Potential Values

	Ammonia	Aniline	Diphenylamine	Phenol
Acidification	1.833153	0	0	0
Ecotoxicity Effect (Aquatic)	0.315757	0.02334	0.583193	0.069072
Ecotoxicity Effect (Terrestrial)	1.019422	1.42719	0.178399	1.125544
Greenhouse Enhancement	0	0	0	0
Human Toxicity Effect (Air)	4.66E-05	8.58E-05	0.000163	8.58E-05
Human Toxicity Effect (Soil)	1.019422	1.42719	0.178399	1.125544
Human Toxicity Effect (Water)	4.66E-05	8.58E-05	0.000163	8.58E-05
Ozone Depletion	0	0	0	0
Photochemical Oxidant Formation	0	0	0	0

The program uses the data entered by the user to evaluate these indices and then displays the 'Index Calculations' window shown in Figure 88. The indices on the left-hand side are the indices based on the generation of potential environmental impacts, and the indices on the right-hand side are the indices based on the emission of impacts. Each index is accompanied by a Help button. Clicking on the 'Help' displays more information about that particular index at the bottom of the screen. The program also calculates the pollution index values for each of the individual streams. To see these values, click on the 'Show WAR algorithm' button. The program now displays the 'Waste Reduction Algorithm' window shown in Figure 89.

In Figure 89, the table on the left-hand side shows the pollution index values for all the input and output streams in the aniline process. A comparison of these values can help in identifying streams with high pollution content. In Figure 89, it can be seen that the pollution index values are zero for all the streams except streams s03, the ammonia feed, s04, the phenol feed, s17, the gaseous purge, and s24, the water product. This shows that the two feed streams are the main source of pollutant emissions into the environment and need special attention.

Pollution Index Program - [Index Calculations]
Process
Indices based on Generation of Potential Environmental Impact
Indices based on Emission of Potential Environmental Impact
Total rate of Impact Generation
-1086.0774195
Impact / Time
Help
Total rate of Impact Emission
155.646526752
Impact / Time
Help
Specific Impact Generation
-0.2967689609
Impact / Product
Help
Specific Impact Emission
4.25303139910
Impact / Product
Help
Rate of Generation of Pollutants per unit product
0.91145065092
Mass Pollutants / Mass of products
Help
Rate of Emission of Pollutants per unit product
10.1318466804
Mass Pollutants / Mass of products
Help
Help on the selected Index :
This index gives the rate at which the process generates potential environmental impact. It is equal to the difference between the total potential impact leaving the system and the total potential impact entering the system. The potential impact of products is taken to be zero
Show WAR algorithm
Back to Stream Data

Figure88. The Index Calculations Window

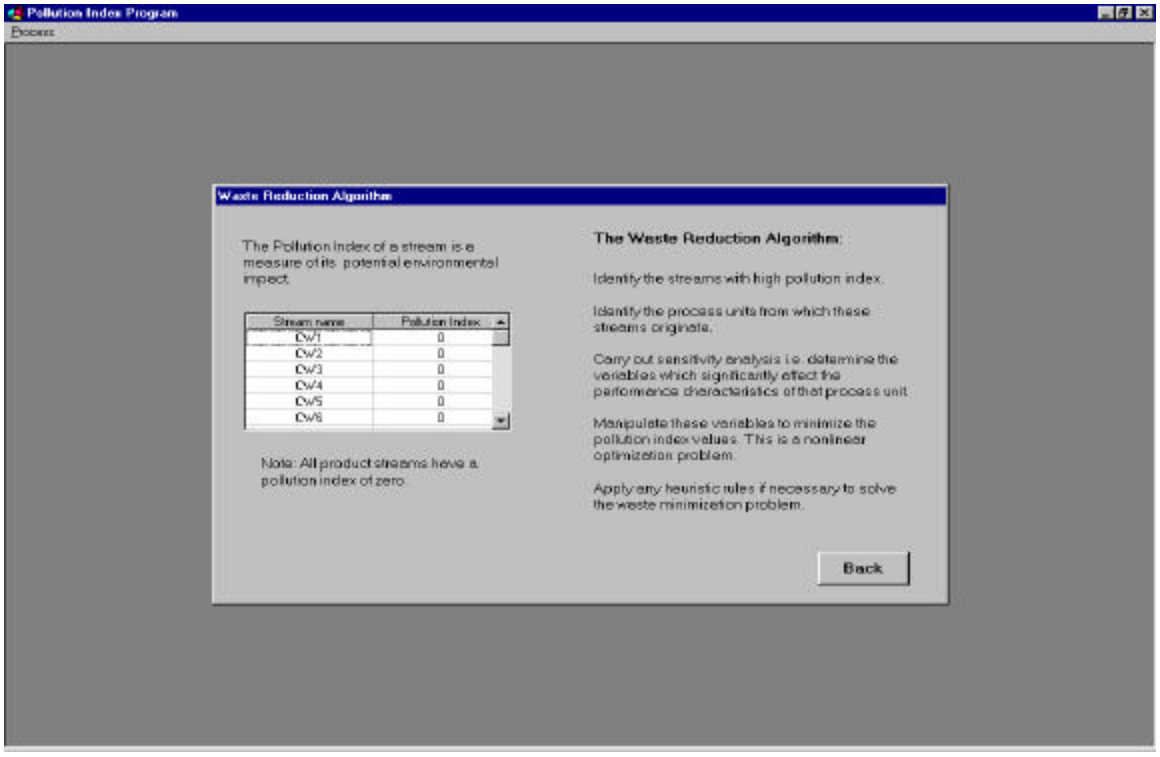

Pollution Index Program
Process
Waste Reduction Algorithm
The Pollution Index of a stream is a measure of its potential environmental impact.
Stream name
Pollution Index
CW1
CW2
CW3
CW4
CW5
CW6
Note: All product streams have a pollution index of zero
The Waste Reduction Algorithm:
Identify the streams with high pollution index.
Identify the process units from which these streams originate.
Carry out sensitivity analysis i.e. determine the variables which significantly effect the performance characteristics of that process unit.
Manipulate these variables to minimize the pollution index values. This is a nonlinear optimization problem.
Apply any heuristic rules if necessary to solve the waste minimization problem.
Back

Figure89. The Waste Reduction Algorithm Window

The right side of the 'Waste Reduction Algorithm' window shows the important steps of WAR algorithm, which gives a systematic way of approaching the waste minimization problem. The back button can be used to go back to the previous screens and make changes in the data. Click on the back button until you reach the process screen shown in Figure 85. Let us save the information entered so far by clicking on the 'Save' button in the 'Process' menu. The program displays the 'Save the model as' dialog box shown in Figure 90. The pollution index program stores the model as a file with '.pnd' extension. Let us save this model as 'aniline.pnd' in the Examples subdirectory of the program folder.

This concludes the implementation of the Pollution Index program in the Advanced Process Analysis System. Click the 'Exit' button in the process menu to return to the Advanced Process Analysis Desk. The next section explains the use of the Chemical Reactor Analysis program.

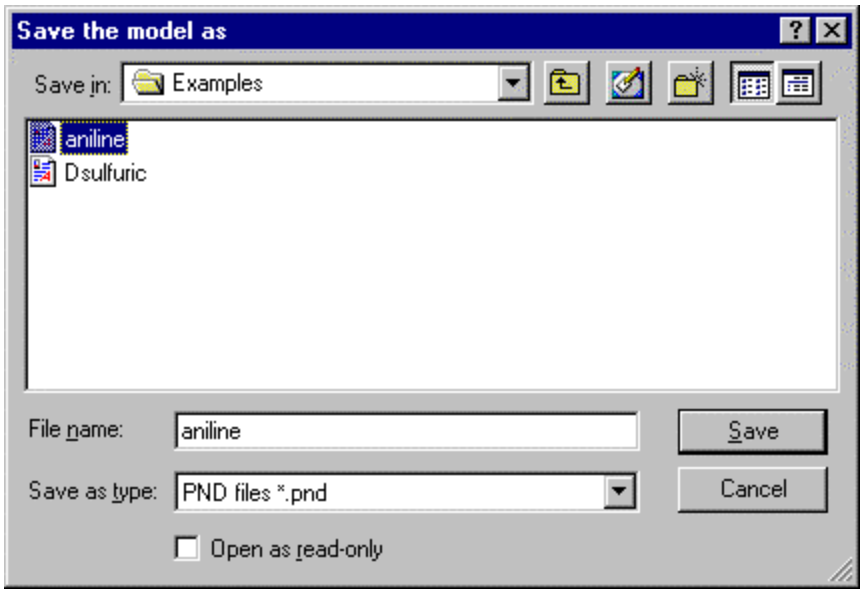


Figure 90 The Save As Window

IX. USING CHEMICAL REACTOR ANALYSIS PROGRAM

The chemical reactor program is an integral part of the Advanced Process Analysis System, and the reactor feed flowrates and compositions are provided to the program from the database. This section presents the screen images of the program with the aniline process model. This will demonstrate how the reactor analysis program is integrated in the Advanced Process Analysis System.

Upon clicking on the 'Reactor Analysis' button on the Advanced Process Analysis Desk shown in Figure 9, the 'Reactor Analysis Model Information' window is displayed. This window is shown in Figure 91.

Since we are using the Reactor Analysis program for the first time, click on the 'New Model' button. Once the 'New Model' button is clicked, the FlowSheet window of the Reactor Analysis program is displayed. This window is shown in Figure 92. The flowsheet diagram for the aniline process model is shown in this window along with a list of units in the model. Choose the reactor unit by clicking on the unit in the flowsheet or from the list. Let us choose the reactor in the model. The selected reactor unit name 'CRV-100' appears in the text box. Clicking the 'Close' button closes this window and displays the Reactor Analysis Main window.

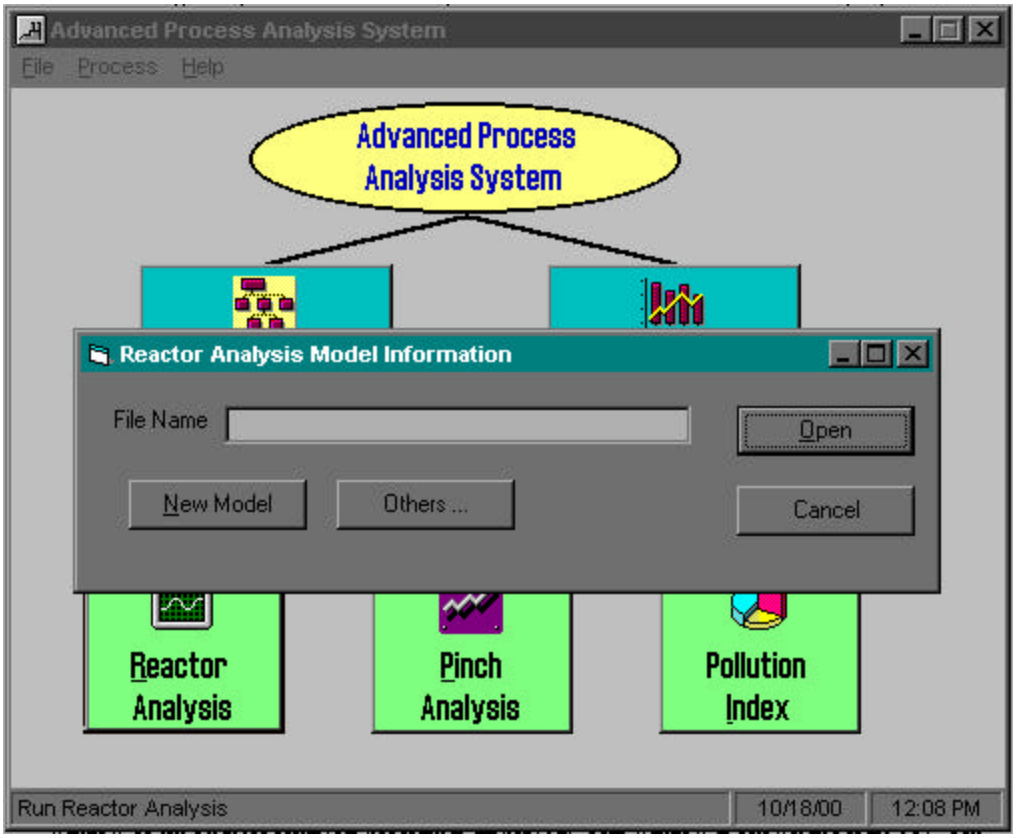


Figure 91. The Reactor Analysis Model Information Window

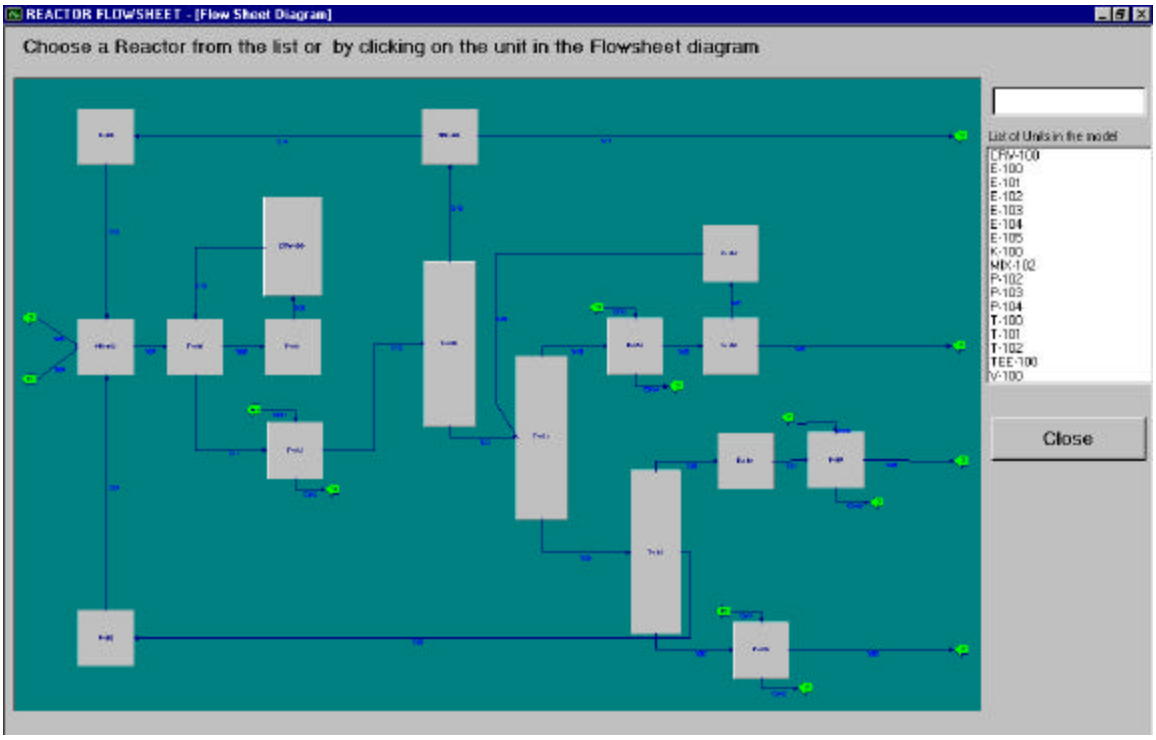

REACTOR FLOWSHEET - [Flow Sheet Diagram]
Choose a Reactor from the list or by clicking on the unit in the Flowsheet diagram
List of Units in the model
Close

Figure 92: Flowsheet Window

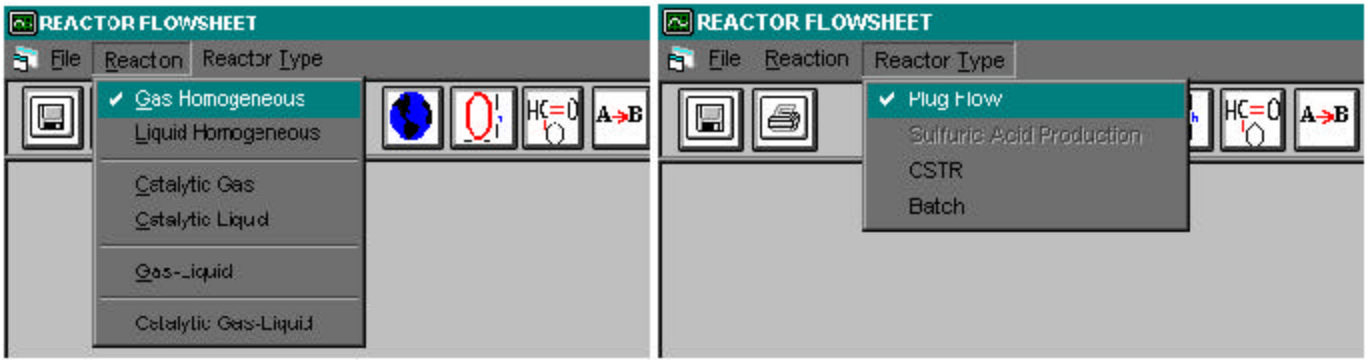


Figure 93: Reaction and Reactor Type Menus

The phase of the reaction should be selected from the 'Reaction' menu, which is shown in Figure 93. Let us choose 'Gas Homogeneous' as the phase of the reaction. Next we have to choose the reactor type from the 'Reactor Type' menu which is also shown in Figure 93. Let us choose 'Plug Flow' as the type of reactor.

Let us proceed to enter the global options. Click on the 'Global Options' icon in the main window to open the Global Options window, which is show in Figure 94. Let us enter the number of reactions to be 3, the number of species to be 7, the inlet temperature needs to be 725 and the inlet pressure to be 245.

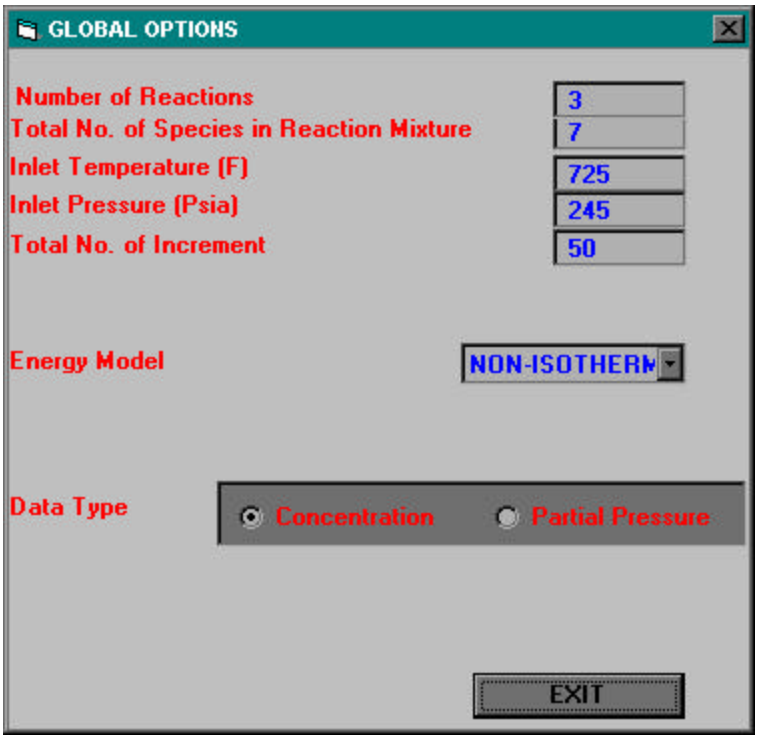


Figure 94. Global Options Window

Choose the Energy Model to be 'Non-Isothermal' from the list. Let the Total Number of Increments be 50. Click on the 'Close' button to close this window and return to the main window.

Let us proceed to the 'Reactant Properties' step. Click on the 'Reactants' icon on the toolbar of the main window to open the Reactant Properties window, which is shown in Figure 95. There are seven components in the reacting gases of CRV-100. These are hydrogen, nitrogen, ammonia, water, phenol, aniline and diphenylamine. These components with their molecular weights and heat capacity coefficients are automatically retrieved from FlowSim.

The table 'Variables' on the right-hand side shows the list of all the measured and unmeasured variables in the aniline model. The value corresponding to the selected variable is shown below the table. Similarly, the list of parameters and constants in the model can be viewed by choosing 'Parameters' and 'Constants' respectively from the list. The value of the selected variable can be loaded as the molecular weight or the heat capacities of a particular species. To do this, click on the grid cell where you want the value to be loaded. Select the variable (or parameter or constant) and then click on the button 'Load Value'.

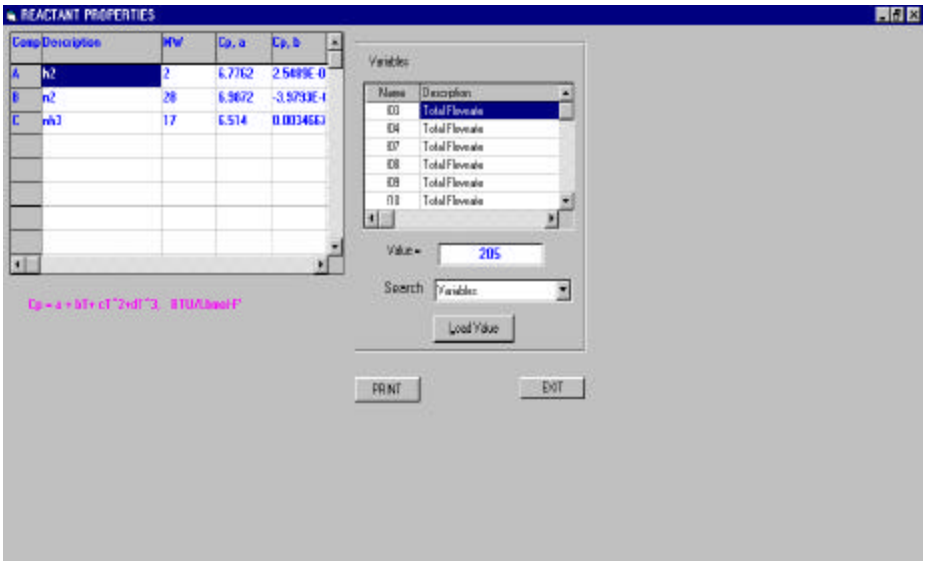


Figure 95. Reactant Properties Window

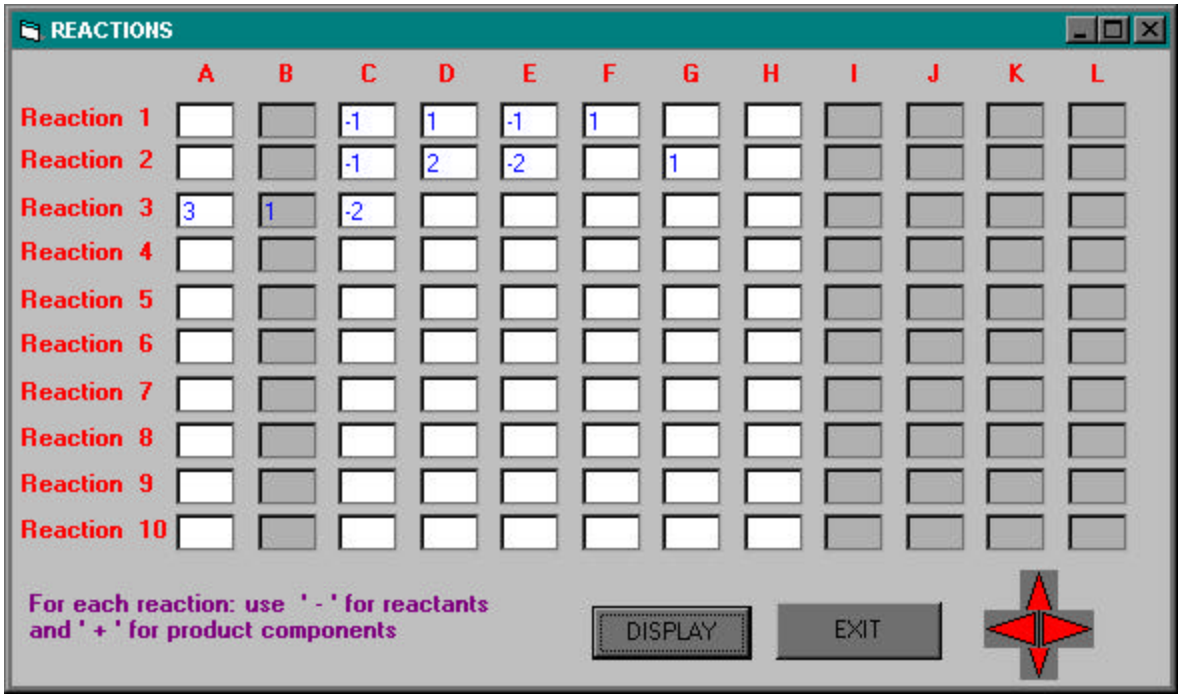


Figure 96. Stoichiometry Window

After the molecular weights and heat capacities for all seven species have been entered, click on the 'Close' button to return to the main window. Clicking on the 'Stoichiometry' icon in the toolbar of the main window opens up the Stoichiometry window. The Stoichiometry window is shown in Figure 96. The reaction stoichiometry coefficients can be entered in this window.

A negative stoichiometric coefficient indicates that this component is acting as a reactant species for the current reaction, while a positive coefficient indicates a reaction product. In Reaction 1 of Figure 98, the coefficient for C (NH_3) is -1, the coefficient for E (phenol) is -1, the coefficient for F (aniline) is 1, and the coefficient for D (H_2O) is 1.

Clicking on the 'Display' button in the Stoichiometry window opens the Reaction Stoichiometry window. The reactions for the given stoichiometric coefficients can be viewed in the form of equations in the Reaction Stoichiometry window. The Reaction Stoichiometry Equations window is shown in Figure 97.

Proceed to the next window by clicking on the 'Rate' icon in the toolbar. The window displayed is the 'Reaction Rate' window. This is shown in Figure 101. The first equation in the window represents the rate expression for the aniline reaction. Cc, Cd, Ce and Cf represent the concentrations of NH_3, H_2O, phenol and aniline, respectively. The rate exression is to be entered by filling in the powers of these concentration terms.

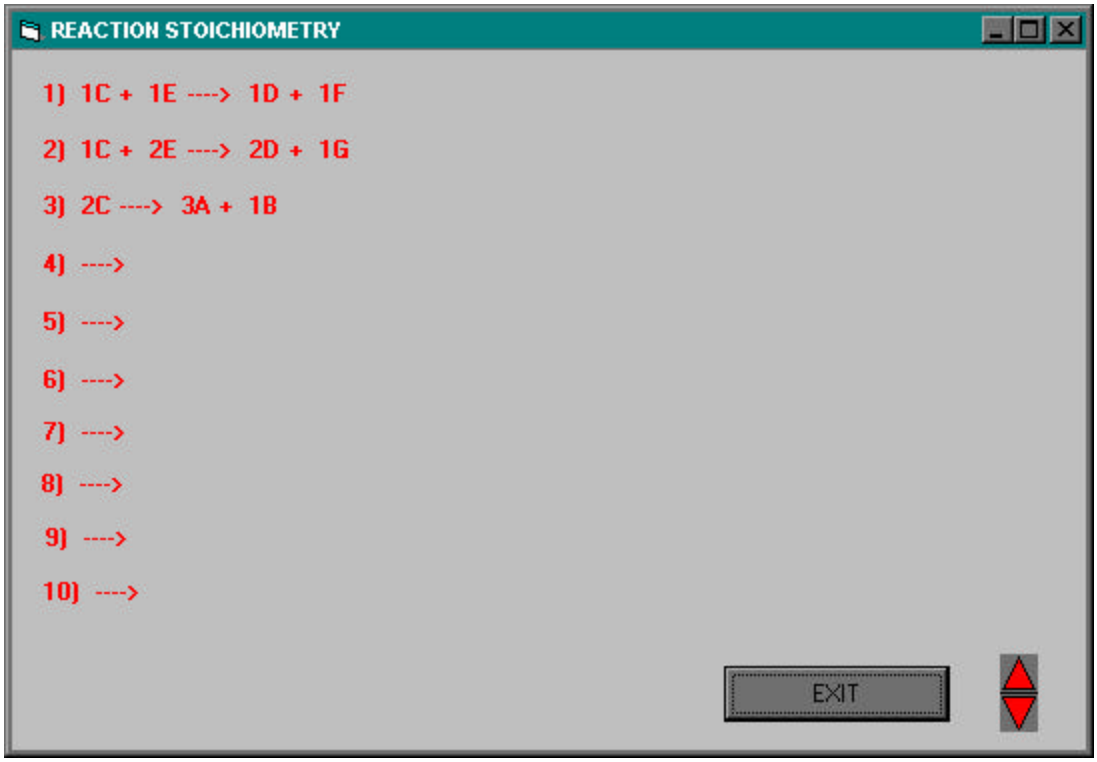


Figure 97 . The Reaction Stiochiometry Equations Window

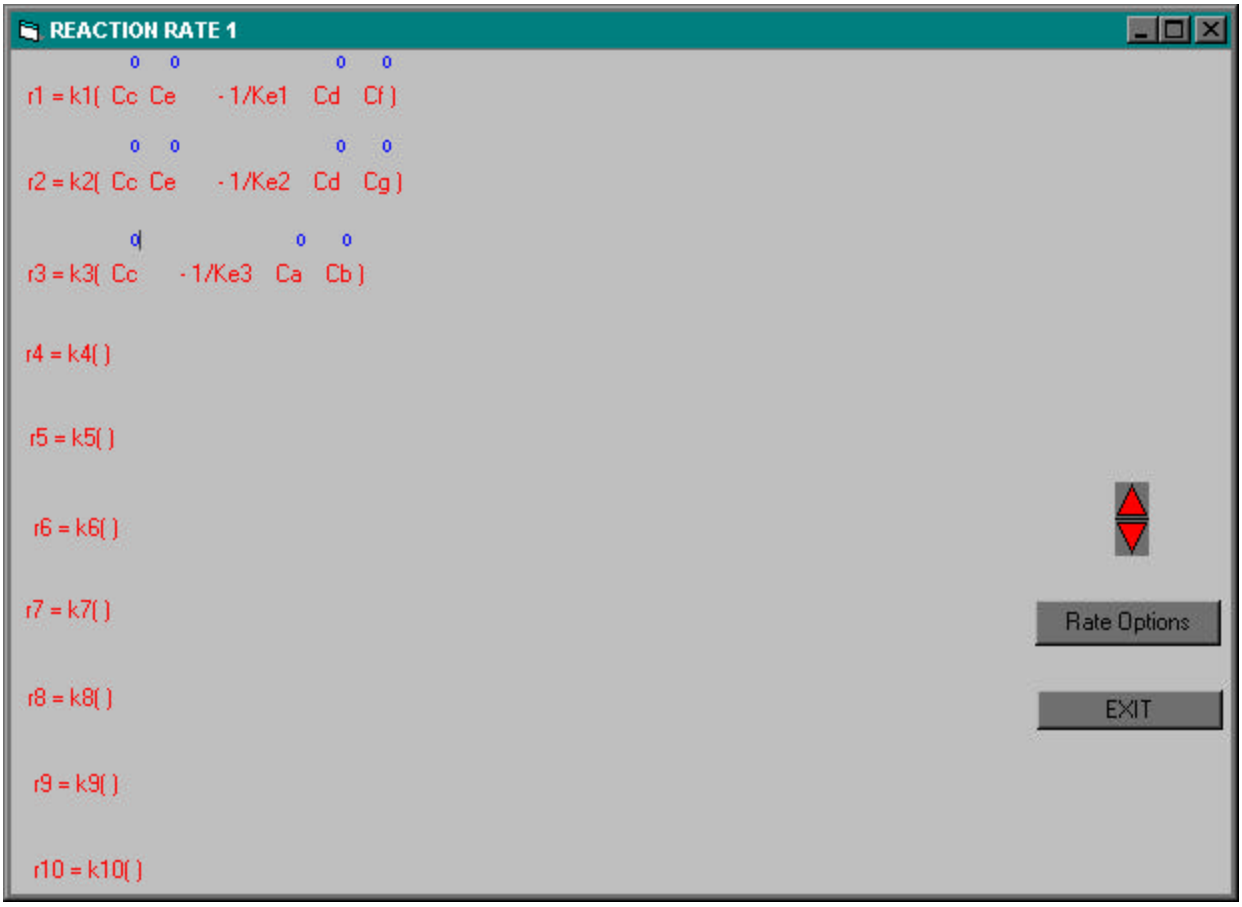

REACTION RATE 1
r1 = k1(Cc^0 Ce^0 - 1/Ke1 Cd^0 Cf^0)
r2 = k2(Cc^0 Ce^0 - 1/Ke2 Cd^0 Cg^0)
r3 = k3(Cc^0 - 1/Ke3 Ca^0 Cb^0)
r4 = k4( )
r5 = k5( )
r6 = k6( )
r7 = k7( )
r8 = k8( )
r9 = k9( )
r10 = k10( )
Rate Options
EXIT

Figure98. The Reaction Rate Window

Next, let us enter the order of each reaction with respect to each component that contributes to the reaction. Forward and reverse reaction orders can be entered in this window. Let us enter the reaction orders for the three reactions in the Reaction Rate window. Let us enter 1 as the reaction order for 'Ce' in the first reaction. Enter 1 as the reaction order for 'Ce' in the second reaction. Finally, enter 2 as the reaction order for 'Cc' in the third reaction. The Reaction Rate window with this information is shown in Figure 99.

Click on the 'Rate Options' button in the Reaction Rate window to enter the reaction rates basis. Each reaction rate should be expressed based on a formation or depletion of a component that appears in the stoichiometry of the reaction as a reactant or as a product. Let us enter the reaction rates for the two reactions as 'F', 'G', and '-C' as shown in Figure 100.

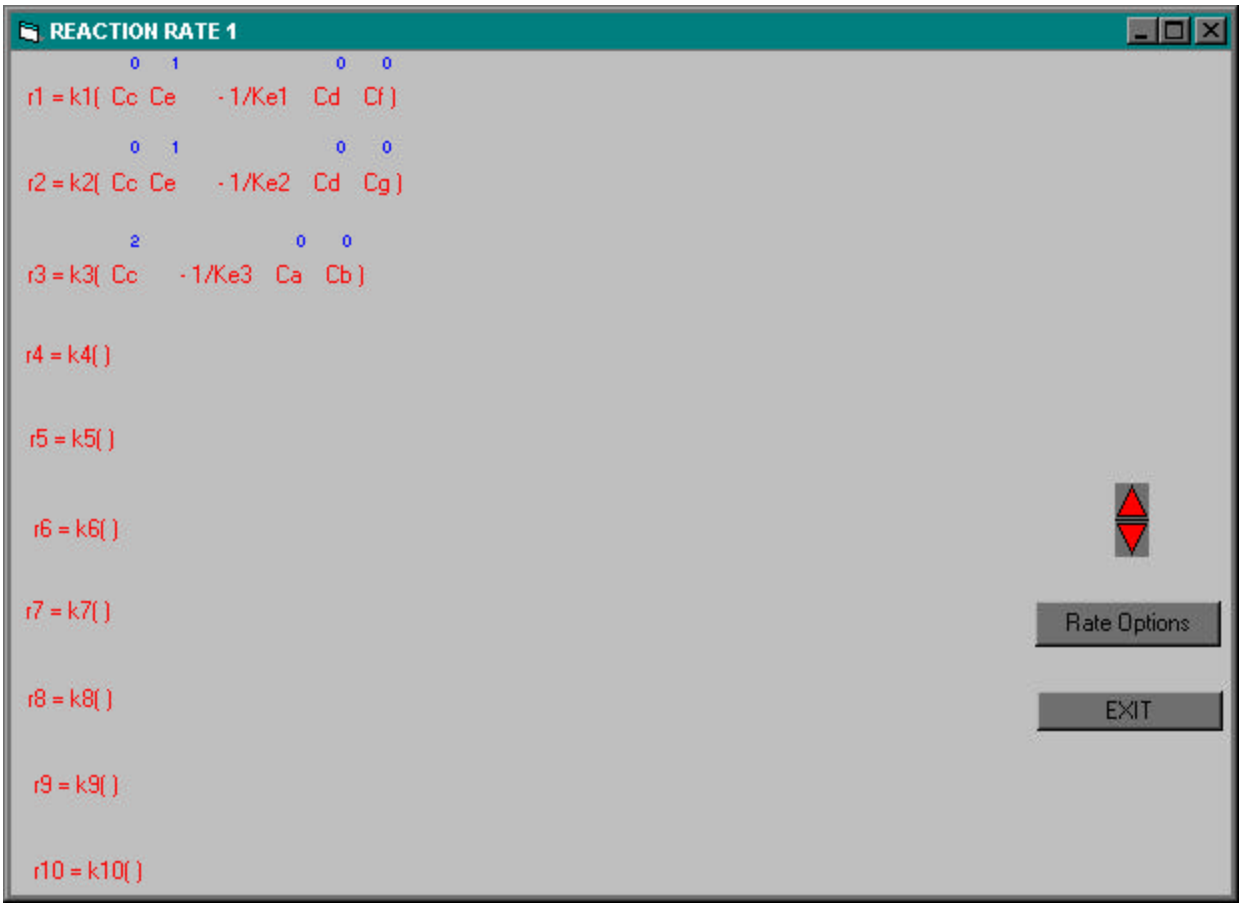

REACTION RATE 1
r1 = k1(Cc^0 Ce^1 - 1/Ke1 Cd^0 Cf^0)
r2 = k2(Cc^0 Ce^1 - 1/Ke2 Cd^0 Cg^0)
r3 = k3(Cc^2 - 1/Ke3 Ca^0 Cb^0)
r4 = k4( )
r5 = k5( )
r6 = k6( )
r7 = k7( )
r8 = k8( )
r9 = k9( )
r10 = k10( )
Rate Options
EXIT

Figure 99. Reaction Rate Window

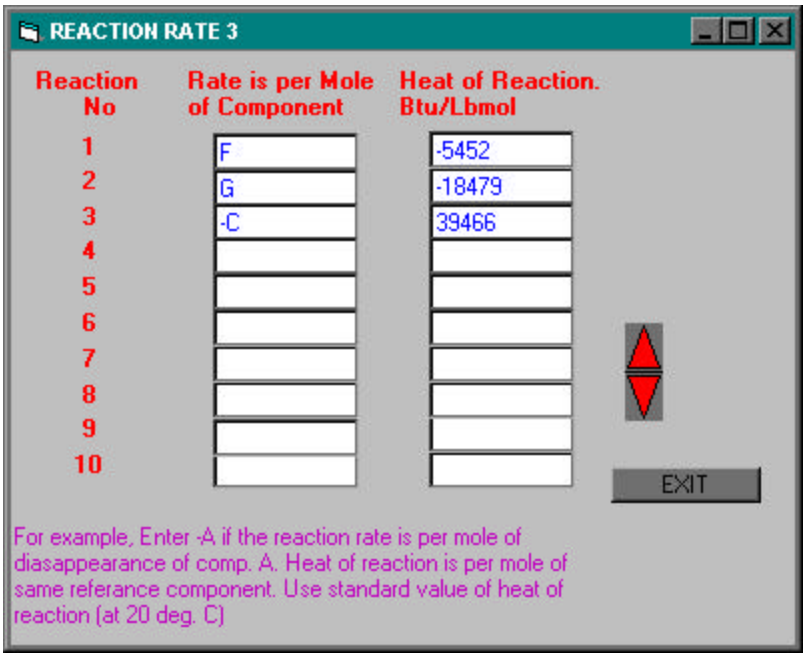
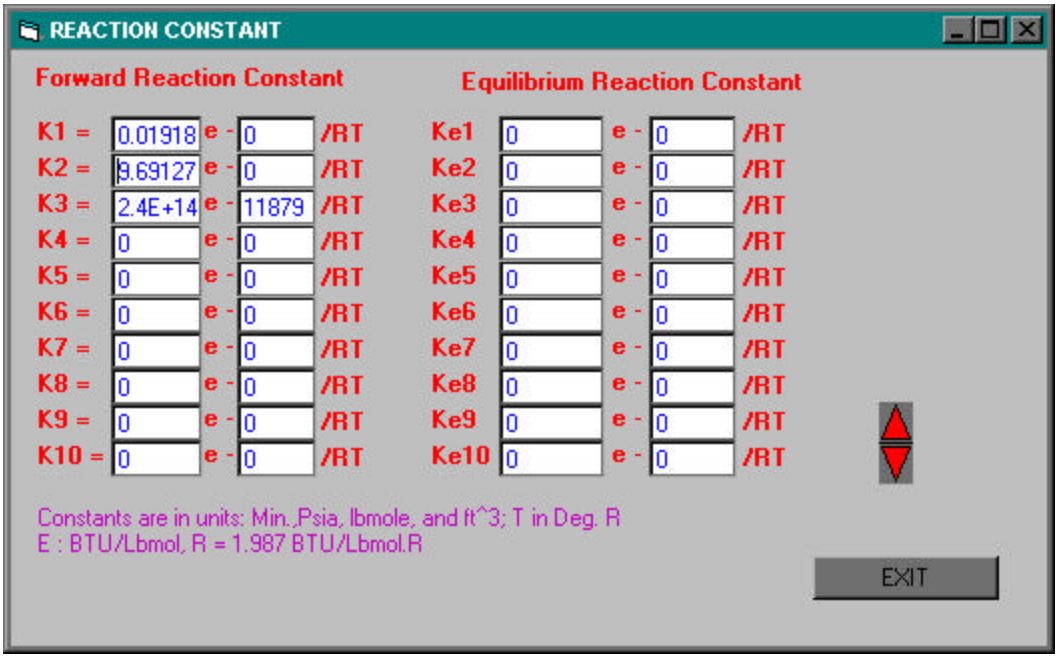

REACTION RATE 3
Reaction No
Rate is per Mole of Component
Heat of Reaction. Btu/Lbmol
1 F -5452
2 G -18479
3 -C 39466
4
5
6
7
8
9
10
EXIT
For example, Enter -A if the reaction rate is per mole of diasappearance of comp. A. Heat of reaction is per mole of same referance component. Use standard value of heat of reaction (at 20 deg. C)

Figure 100. Reaction Rate Options Window


REACTION CONSTANT
Forward Reaction Constant
Equilibrium Reaction Constant
K1 = 0.01918 e - 0 /RT
K2 = 9.69127 e - 0 /RT
K3 = 2.4E+14 e - 11879 /RT
K4 = 0 e - 0 /RT
K5 = 0 e - 0 /RT
K6 = 0 e - 0 /RT
K7 = 0 e - 0 /RT
K8 = 0 e - 0 /RT
K9 = 0 e - 0 /RT
K10 = 0 e - 0 /RT
Ke1 0 e - 0 /RT
Ke2 0 e - 0 /RT
Ke3 0 e - 0 /RT
Ke4 0 e - 0 /RT
Ke5 0 e - 0 /RT
Ke6 0 e - 0 /RT
Ke7 0 e - 0 /RT
Ke8 0 e - 0 /RT
Ke9 0 e - 0 /RT
Ke10 0 e - 0 /RT
Constants are in units: Min.,Psia, lbmole, and ft^3; T in Deg. R
E : BTU/Lbmol, R = 1.987 BTU/Lbmol.R
EXIT
Figure 101. Reaction Rate Constants Window

Click the 'Exit' button to return to the Reaction Rate window. Click on the 'Exit' button in the Reaction Rate window to return to the main window. Next let us enter the Reaction Rate constants. Click on the 'Reactor Constants' icon in the main window to open the Reaction Rate Constants window.

The forward reaction constant K1 and the equilibrium constant Ke1 may be entered in this window according to an Arrhenius-type equation:

$$K1 = A\, e^{-E/RT}$$
$$Ke1 = Ae1\, e^{-Ee1/RT}$$

Let us enter the forward reaction constants for the first two reactions as 0.0191887 and 9.69127E-05 as shown in Figure 101. The final reaction is temperature dependent as shown by Figure 101. The first constant for the reaction rate in the third equation is 2.4E+14, while the second constant is 118790. Click on the 'Close' button to return to the main window after entering all forward reaction constants and equilibrium constants.

The Reactor Analysis program needs the reactor dimensions such as length, diameter and input volumetric flow rate. To enter this data, click on the 'Reactor Spec' icon in the toolbar of the main window. Clicking on the 'Reactor Spec' button opens the Reactor Specification window. The Reactor Specification window is given in Figure 102. Let us enter 8.5 for the reactor diameter, 85 for reactor length and 586 for the input flow rate.

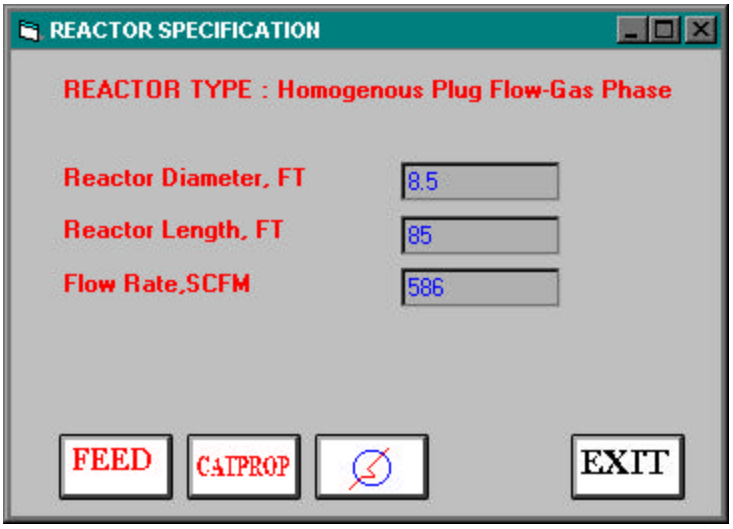


Figure 102. The Reaction Specification Window

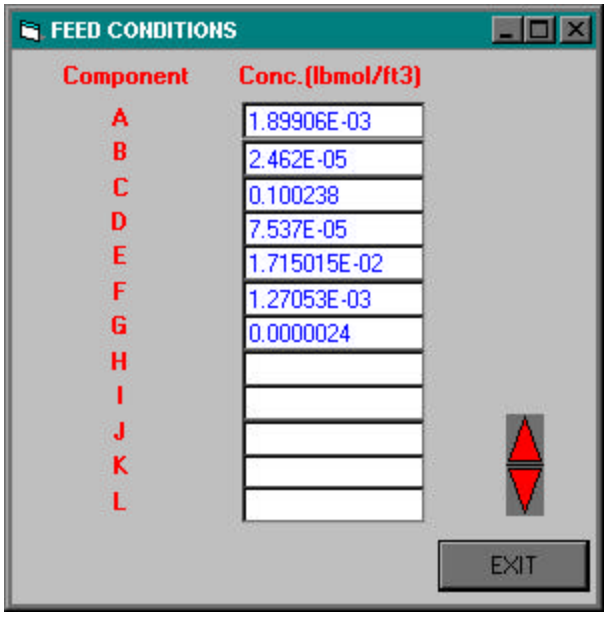


Figure 103. Initial Feed Composition Window

Clicking on the 'FEED' button in this window opens the Feed Composition window. The initial feed composition for the components are entered here. Let us enter the initial feed composition for the components A, B, C, D, E, F and G as given in Figure 103.

Click on the 'Exit' button to return to the Reactor Specification window. Click on the 'Close' button in the Reactor Specification window to return to the main window. All the information required by the Reactor Analysis program has been entered.

The information can also be entered step by step starting from the Global Options window and proceeding through the other windows in a sequential fashion using the 'Next' and 'Back' icons in the main window.

To run the model, click on the 'Run' icon in the toolbar of the main window. The total reactor length will be divided by the number of increments (as specified in Figure 95) and the calculations will be performed for each increment. The results will be displayed graphically as shown in Figure 104.

Figure 104 shows the graph plotted with the concentration versus length of the reactor. Similarly the graph can be plotted for temperature, pressure or conversion. These four variables (concentration, temperature, pressure and conversion) can also be plotted versus or volume of the reactor.

The results can also be viewed in a tabular form by clicking on the 'Data Grid' option provided in the left bottom corner of the main window. The results in the tabular form are shown in Figure 105. The data can be displayed as a function of reactor length or volume.

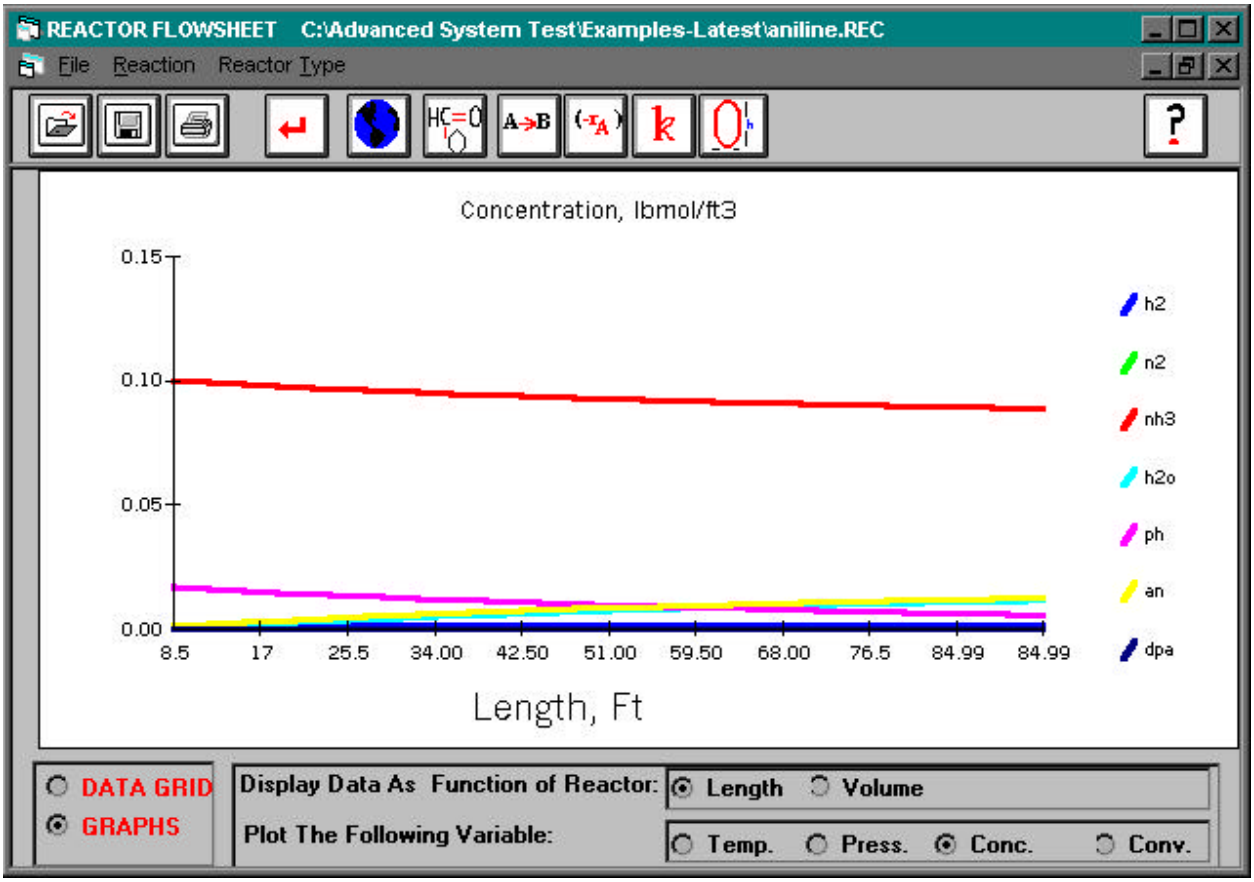
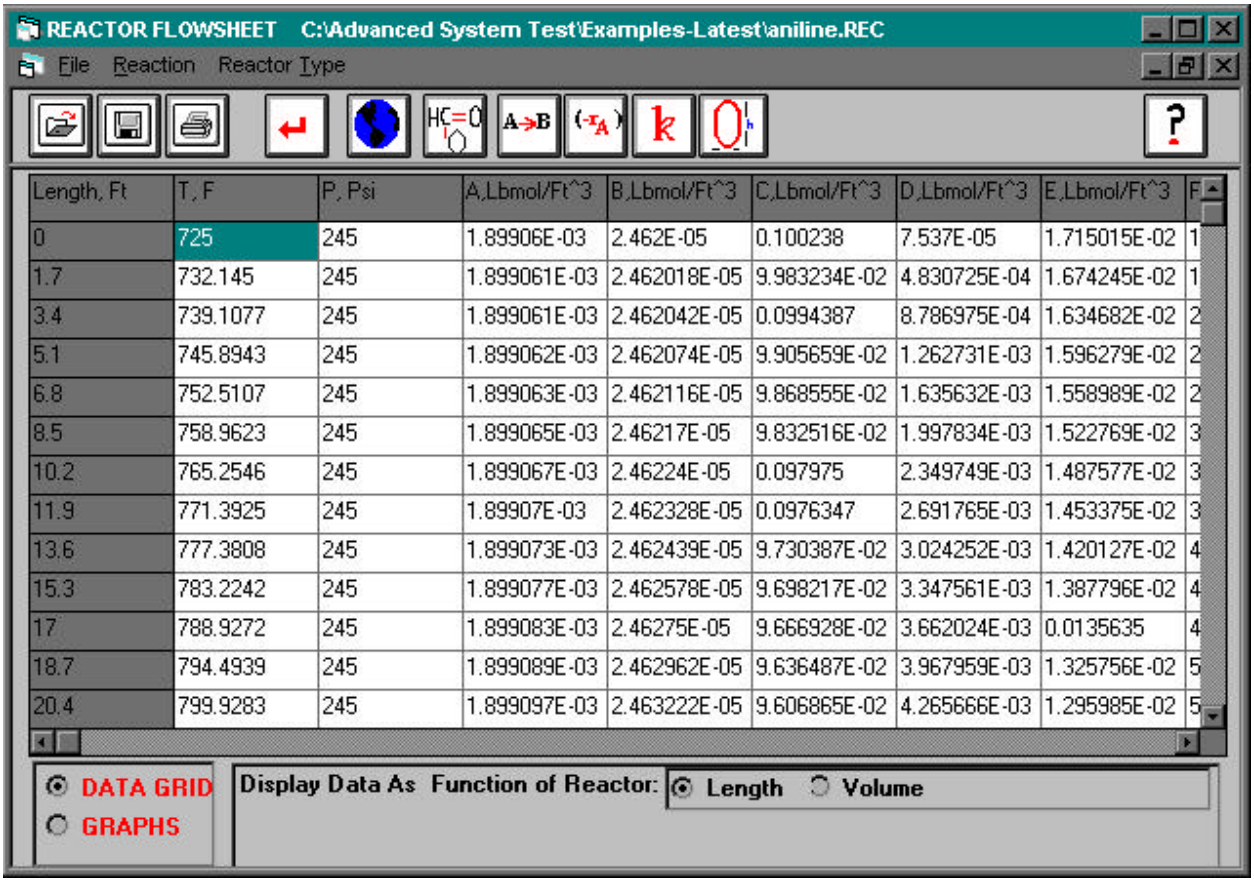


Figure 104. Results in Graphical Form



Length, Ft	T, F	P, Psi	A,Lbmol/Ft^3	B,Lbmol/Ft^3	C,Lbmol/Ft^3	D,Lbmol/Ft^3	E,Lbmol/Ft^3	F
0	725	245	1.89906E-03	2.462E-05	0.100238	7.537E-05	1.715015E-02	1
1.7	732.145	245	1.899061E-03	2.462018E-05	9.983234E-02	4.830725E-04	1.674245E-02	1
3.4	739.1077	245	1.899061E-03	2.462042E-05	0.0994387	8.786975E-04	1.634682E-02	2
5.1	745.8943	245	1.899062E-03	2.462074E-05	9.905659E-02	1.262731E-03	1.596279E-02	2
6.8	752.5107	245	1.899063E-03	2.462116E-05	9.868555E-02	1.635632E-03	1.558989E-02	2
8.5	758.9623	245	1.899065E-03	2.46217E-05	9.832516E-02	1.997834E-03	1.522769E-02	3
10.2	765.2546	245	1.899067E-03	2.46224E-05	0.097975	2.349749E-03	1.487577E-02	3
11.9	771.3925	245	1.89907E-03	2.462328E-05	0.0976347	2.691765E-03	1.453375E-02	3
13.6	777.3808	245	1.899073E-03	2.462439E-05	9.730387E-02	3.024252E-03	1.420127E-02	4
15.3	783.2242	245	1.899077E-03	2.462578E-05	9.698217E-02	3.347561E-03	1.387796E-02	4
17	788.9272	245	1.899083E-03	2.46275E-05	9.666928E-02	3.662024E-03	0.0135635	4
18.7	794.4939	245	1.899089E-03	2.462962E-05	9.636487E-02	3.967959E-03	1.325756E-02	5
20.4	799.9283	245	1.899097E-03	2.463222E-05	9.606865E-02	4.265666E-03	1.295985E-02	5

Figure 105. Reactor Analysis Results in Tabular Form.

Save the file as a '.REC' file using the 'Save As' option in the File menu of the main window. Exit the program by clicking on the 'End' option in the File menu of the main window. This concludes the use of the reactor analysis program for the example problem.

XI. OPTIMIZATION SOLVER-GAMS

A. Compilation Output (Brooke, et al., 1996)

The compilation output is produced during the initial check of the program, and it is often referred to as a compilation. It includes two or three parts: the echo print of the program, an explanation of any errors detected, and the symbol reference maps. The echo print of the program is always the first part of the output file. If errors had been detected, the explanatory messages would be found at the end of the echo print. The echo print of the GAMS program for the economic optimization of the contact process is included in the GAMS output file in Section X.

The symbol reference maps follow the echo print, and they include the symbol cross-reference and the symbol-listing map. These are extremely useful if one is looking into a model written by someone else, or if one is trying to make some changes in their own model after spending time away from it. The symbol cross reference lists the identifiers (symbols) in the model in alphabetical order, identifies their type, shows the line numbers where the symbols appear, and classifies each appearance. The complete list of data types is given in Table 8. Next in the listing is a list of references to the symbols, grouped by reference type and identified by the line number in the output file. The actual references can then be found by referring to the echo print of the program, which has line numbers on it. The complete list of reference types is given in Table 9. The symbol reference maps do not appear in the output files by default. However, it can be included in the output files by changing the default setting in Output File Format Specification window.

Table 8 A List of Data Types

Entry in symbol reference table	GAMS data type
SET	set
PARAM	parameter
VAR	variable
EQU	equation
MODEL	model

B. Execution Output

The execution output follows the compilation output and is also found in the GAMS output file. If a display statement is present in the GAMS program, then data requested by the display statement is produced in the execution output while GAMS performs data manipulations. Also, if errors are detected because of illegal data operations, a brief message indicating the cause and the line number of the offending statement, will appear in the execution output. The execution output will be shown in the GAMS output file if a display statement is present in the GAMS

program (which requests the display of the value of a variable) or if an execution error is encountered.

Table 9 A List of Reference Types

Reference	Description
DECLARED	This is where the identifier is declared as to type. This must be the first appearance of the identifier.
DEFINED	This is the line number where an initialization (a table or a data list between slashes) or symbol definition (equation) starts for the symbol.
ASSIGNED	This is when values are replaced because the identifier appears on the left of an assignment statement.
IMPL-ASN	This is an "implicit assignment": an equation or variable will be updated as a result of being referred to implicitly in a solve statement.
CONTROL	This refers to the use of a set as the driving index in an assignment, equation, loop or other indexed operation (sum, prod, smin or smax).
REF	This is a reference: the symbol has been referenced on the right of an assignment in a display, in an equation, or in a model or solve statement.

C. Output produced by a Solve Statement (Brooke, et al., 1996)

The output triggered by a solve statement includes the equation listing, the column listing, the model statistics, solver report, the solution listing, report summary, and file summary as shown in the GAMS output file in Section X. All of the output produced as a result of a SOLVE statement is labeled with a subtitle identifying the model, its type, and the line number of the solve statement.

The first list in the output produced by the SOLVE statement is the Equation Listing, which is marked with that subtitle in the output file. The Equation Listing is an extremely useful debugging aid. It shows the variables that appear in each constraint, and what the individual coefficients and right-hand-side value evaluate to after the data manipulations have been made. Normally, the first three equations in every block are listed. Most of the listing is self-explanatory. The name, text, and type of constraints are shown. The four dashes are useful for mechanical searching. All terms that depend on variables are collected on the left, and all the constant terms are combined into one number on the right, with any necessary sign changes made. For example, a equation "x + 5y - 10z +20 =e= 0" is rearranged as: "x + 5y - 10z =e= -20". Four places of decimals are shown if necessary, but trailing zeroes following the decimal point are suppressed. E-format is used to prevent small numbers being displayed as zero. By

default, the equation listing will not appear in the output file unless specified by the user in the Output File Format Specification Window.

The general format in the equation listing was described above. However, the nonlinear terms in an equation are treated differently from the linear terms. If the coefficient of a variable in the Equation Listing is enclosed in parentheses, then the variable corresponding to this coefficient is nonlinear in the constraint equation, and the value of the coefficient depends on the activity levels of one or more of the variables. This coefficient is not algebraic, but it is the partial derivative of each variable evaluated at their current level values (initial points).

For an equation: $x + 2y^3 +10 =e= 0$ with current level values $x = 2$ and $y = 1$, this equation is listed in the equation listing as: $x + (6)\ y =e= -12$, where the coefficient of y is the partial derivative of the equation with respect to y evaluated at y=1, i.e., $6y^2 = 6$. The right hand side coefficient, -12, is the sum of constant in the equation, 10, and the constant, 2, from the linearization of the nonlinear term $2y^3$ using Taylor expansion evaluated at $y = 1$. x in this equation is linear, and its coefficient is shown as 1 without the parentheses.

Next, the column listing gives the individual coefficients sorted by column rather than by row. The default shows the first three entries for each variable, along with their bound and level values. The format for the coefficients is the same as in the equation listing, with the nonlinear ones enclosed in parentheses and the trailing zeroes dropped. The order in which the variables appear is the order in which they were declared.

The final information generated while a model is being prepared for solution is the statistics block to provide details on the size and nonlinearity of the model. The status for the solver (the state of the program) and the model (what the solution looks like) are characterized in solver status and model status. The model status and solver status are listed in Table 10 and Table 11, respectively.

The next section is the solver report, which is the solve summary particular to the solver program that has been used. Also, there will be diagnostic messages in plain language if anything unusual was detected, and specific performance details as well. In case of serious trouble, the GAMS listing file will contain additional messages printed by the solver, which may help, identify the cause of the difficulty.

Solution listing is a row-by-row then column-by-column listing of the solutions returned to GAMS by the solver program. Each individual equation and variable is listed with four pieces of information. The four columns associated with each entry are listed in Table 12. For variables, the values in the LOWER and UPPER columns refer to the lower and upper bounds. For equations, they are obtained from the (constant) right-hand-side value and from the relational type of the equation. EPS means very small or close to zero. It is used with non-basic variables whose marginal values are very close to, or actually, zero, or in nonlinear problems with super-basic variables whose marginal values are zero or very close to it. A superbasic variable is the one between its bounds at the final point but not in the basis.

For models that do not reach an optimal solution, some constraints may be marked with the flags shown in Table 13. The final part of solution listing is the report summary marked with four asterisks. It shows the count of rows or columns that have been marked INFES, NOPT, UNBND. The sum of infeasibilities will be shown if the reported solution is infeasible. The error count is only shown if the problem is nonlinear. The last piece of the output file is the file summary, which gives the names of the input and output disk files. If work files have been used, they will be named here as well.

D. Error Reporting

The last part in the output file is error reporting. All the comments and descriptions about errors have been collected into this section for easy reference. Errors are grouped into the three phases of GAMS modeling in the on-line optimization system: compilation, execution and model generation (which includes the solution that follows). They will be illustrated in the section, "Error Reporting".

Table 10 A List of Model Status in GAMS Output Files

Model status	Meaning
1. Optimal	This means that the solution is optimal. It only applies to linear problems or relaxed mixed integer problems (RMIP).
2. Locally Optimal	This message means that a local optimal for nonlinear problems, since all that can guarantee for general nonlinear problems is a local optimum.
3. Unbounded	That means that the solution is unbounded. It is reliable if the problem is linear, but occasionally it appears for difficult nonlinear problem that lack some strategically paced bounds to limit the variables to sensible values.
4. Infeasible	This means that he linear problem is infeasible.
5. Locally Infeasible	This message means that no feasible point could be found for the nonlinear problem from the given starting point. It does not necessarily mean that no feasible point exists.
6. Intermediate Infeasible	The current solution is not feasible, the solver program stopped, either because of a limit (iteration or resource), or some sort of difficulty.
7. Intermediate Nonoptimal	This is again an incomplete solution, but it appears to be feasible.
8. Integer Solution	An integer solution has been found to a MIP (mixed integer problem).
9. Intermediate Noninteger	This is an incomplete solution to a MIP. An integer solution has not yet been found.
10. Integer	There is no integer solution to a MIP. This message should be reliable.
11.Error Unknown, Error no Solution	There is no solution in either of these cases.

Table 11 A List of Solver Status in GAMS Output Files

Solver status	Meaning
1. Normal Completion	This means that the solver terminated in a normal way: i.e., it was not interrupted by an iteration or resource limit or by internal difficulties. The model status describes the characteristics of the accompanying solution.
2. Iteration Interrupt	This means that the solver was interrupted because it used too many iterations. Use option iterlim to increase the iteration limit if everything seems normal.
3. Resource Interrupt	This means that the solver was interrupted because it used too much time. Use option reslim to increase the time limit if everything seems normal.
4. Terminated by Solver	This means that the solver encountered difficulty and was unable to continue. More detail will appear following the message.
5. Evaluation Error Limit	Too many evaluations of nonlinear terms at undefined values. You should use bounds to prevent forbidden operations, such as division by zero. The rows in which the errors occur are listed just before the solution.
6. Unknown Error Preprocessor(s) Error Setup Failure Error Solver Failure Error Internal Solver Error Error Post-Processor	All these messages announce some sort of unanticipated failure of GAMS, a solver, or between the two. Check the output thoroughly for hints as to what might have gone wrong.

Table 12 A List of Solution Listing Types

Heading in listing file	Description
LOWER	Lower Bound (.lo)
LEVEL	Level Value (.l)
UPPER	Upper Bound (.up)
MARGINAL	Marginal (.m)

Table 13 A List of Constraint Flags

Flag	Description
INFES	The row or column is infeasible. This mark is make for any entry whose LEVEL value is not between the UPPER and LOWER bounds.
NOPT	The row or column is non-optimal. This mark is made for any non-basic entries for which the marginal sign is incorrect, or superbasic ones for which the marginal value is too large.
UNBND	The row or column that appears to cause the problem to be unbounded.

E. GAMS Input Model (Brooke et al., 1996)

The basic components of a GAMS input model include:

- Sets
- Data (Parameters, Tables, Scalar)
- Variables
- Assignment of bounds and/or initial values
- Equations
- Model and Solve statements
- Display/Put statement

The overall content of GAMS output file is:

- Echo Print
- Reference Maps
- Equation Listings
- Status Reports
- Results

E-1. Format for Entering System Information

The GAMS input code generated by the interactive on-line optimization system is based on the information provided by the user. Although the user usually does not need to consider the format of the GAMS program, there are some regulations about the format related to GAMS that must be followed to properly enter information about the plant. The input must be in correct format for an accurate GAMS input file to be generated automatically by the on-line optimization system.

Most of the characters and words are allowable for the input information, however, the letters in the input information are case insensitive. A few characters are not allowed for the input because they are illegal or ambiguous on some machines. Generally, all unprintable and control characters are illegal. Most of the uncommon punctuation characters are not part of the language, but can be used freely. In Table 14, a full list of legal characters is given.
Besides characters, there are some reserved words and non-alphanumeric symbols with predefined meanings in GAMS, which can not be used, in input information. The reserved words and non-alphanumeric symbols are listed in Table 15 and Table 16, respectively.

Table 14 A List of Full Set of Legal Characters for GAMS

A to Z	alphabet	a to z	alphabet	0 to 9	Numerals
&	ampersand	“ ”	double quote	#	pound sign
*	asterisk	=	equals	?	question mark
@	at	>	greater than	;	semicolon
\	back slash	<	less than	‘	single quote
:	Colon	-	minus	/	slash
,	comma	( )	parenthesis		space
$	Dollar	[ ]	square brackets	_	underscore
.	Dot	{ }	braces	!	exclamation mark
+	Plus	%	percent	^	circumflex

Table 15 A List of All Reserved Words for GAMS

abort	ge	Not	smin	if
acronym	gt	Option	sos1	then
acronyms	inf	Options	sos2	else
alias	integer	Or	sum	semicont
all	le	Ord	system	semiint
and	loop	Parameter	table	file
assign	lt	Parameters	using	files
binary	maximizing	Positive	variable	putpage
card	minimizing	Prod	variables	puttl
display	model	Scalar	xor	free
eps	models	Scalars	yes	no
eq	na	Set	repeat	solve
equation	ne	Sets	until	for
equations	Negative	Smax	while	

In the on-line optimization system, numeric values are entered in a style similar to that used in other computer languages. Blanks cannot be used in a number because the system treats a blank as a separator. The common distinction between real and integer data types does not exist. If a number is entered without a decimal point, it is still stored as a real number. In addition, the system uses an extended range arithmetic that contains special symbols for infinity (INF), negative infinity (-INF), undefined (UNDF), epsilon (EPS), and not available (NA) as shown in Table 17. One cannot enter UNDF; it is only produced by an operation that does not have a proper result, such as division by zero. All other special symbols can be entered and used as if they were ordinary numbers.

Table 16 A List of Non-alphanumeric Symbols for GAMS

=l=	--
=g=	++
=e=	**
=n=	

GAMS uses a small range of numbers to ensure that the system will behave in the same way on a wide variety of machines. A general rule is to avoid using or creating numbers with

absolute values greater than 1.0e+20. A number up to 10 significant digits can be entered on all machines, and some machines can even support more than that. However, if a number is too large, it may be treated by the system as undefined (UNDF), and all values derived from it in a model may be unusable. It is recommended to always use INF (or -INF) explicitly for arbitrarily large numbers. When an attempted arithmetic operation is illegal or has undefined results because of the value of arguments (division by zero is the normal example), an error is reported and the result is set to undefined (UNDF). Afterwards, UNDF is treated as a proper data value and does not trigger any additional error messages. Thus, the system will not solve a model if an error has been detected, but it will terminate with an error condition.

The string definition such as the variable's name in the system has to start with a letter followed by more letters or digits. It can only contain alphanumeric characters and up to 10 characters long. The comment to describe the set or element must not exceed 80 characters. Basically, there are five possible types of variables that may be used which are listed in Table 18.

The type of mathematical programming problem must be known before the problem is solved. The on-line optimization system can only solve linear and nonlinear optimization problems. However, GAMS can solve a large number of optimization problems, which are summarized in Table 19.

As the interactive on-line optimization system writes all the required GAMS input files for the user, most of the components in the GAMS input model are automatically formulated from the information provided in the input windows. If the user can follow the explicit rules introduced above, the GAMS input file can be generated automatically. After the user enters all the plant information through the input windows, the GAMS source codes will be generated.

Table 17 A List of Special Symbols for GAMS

Special symbol	Description
INF	Plus infinity. A very large positive number
-INF	Minus infinity. A very large negative number
NA	Not available. Used for missing data. Any operation that uses the value NA will produce the result NA
UNDF	Undefined. The result of an undefined or illegal operation. The user cannot directly set a value to UNDF
EPS	Very close to zero, but different from zero.

Table 18 A List of Types of Variables for GAMS

Keyword	Default Lower Bound	Default Upper Bound	Description
Free (default)	-inf	+inf	No bounds on variables. Both bounds can be changed from the default values by the user
Positive	0	+inf	No negative values are allowed for variables. The upper bound can be changed from the default value by the user
Negative	-inf	0	No positive values are allowed for variables. The user can change the lower bound from the default value.
Binary	0	1	Discrete variable that can only take values of 0 or 1
Integer	0	100	D Discrete variable that can only take integer values between the bounds. Bounds can be changed from the default value by the user

The on-line optimization system will then forward these source codes to the GAMS software. This initiates the execution of GAMS and also creates output files so the user can view the execution in the output window. The execution and the output has been discussed in the previous sections.

Table 19 A List of Types of Models for GAMS

Model Type	Description
LP	Linear programming. No nonlinear terms or discrete (binary or integer) variables.
NLP	Nonlinear programming. There are general nonlinear terms involving only "smooth" functions in the model, but no discrete variables.
DNLP	Nonlinear programming with discontinuous derivatives. Same as NLP, but "non-smooth" functions can appear as well. More difficult to solve than NLP. Not recommended to use.
RMIP	Relaxed mixed integer programming. Can contain discrete variables but the integer and binary variables can be any values between their bounds.
MIP	Mixed integer programming. Like RMIP but the discrete requirements are enforced: the discrete variables must assume integer values between their bounds.
RMINLP	Relaxed mixed integer nonlinear programming. Can contain both discrete variables and general nonlinear terms. The discrete requirements are relaxed. Same difficulty as NLP.
MINLP	Mixed integer nonlinear programming. Characteristics are the same as for RMINLP, but the discrete requirements are enforced.
MCP	Mixed Complementarily Problem
CNS	Constrained Nonlinear System

E-2. Equation Formulation

Besides the rules introduced above, the equations as the main part of the input information have their own specific requirements. The mathematical definitions of equations can be written in one or multiple lines. Blanks can be inserted to improve readability, and expressions can be arbitrarily complicated. The standard arithmetic operations for the equations are listed in Table 20. The arithmetic operations listed in Table 20 are in order of precedence, which determines the order of evaluation in an equation without parentheses. The relational operators in the equations are:

=L= Less than: left hand side (lhs) must be less than or equal to right hand side (rhs)
=G= Greater than: lhs must be greater than or equal to rhs
=E= Equality: lhs must equal to rhs
=N= No relationships enforced between lhs and rhs. This type is rarely used.

Additionally, GAMS provides the numerical relationships and logical operators used to generate logical conditions for evaluating values of True or False. A result of zero is treated as a logical value of False, while a non-zero result is treated as a logical value of True. A complete numerical relationship operators and logical operators are listed in the Table 21 and Table 22, respectively.

Table 20 A List of Standard Arithmetic Operators

Operator	Description
**	Exponentiation
*, /	Multiplication and division
+, -	Addition and subtraction (unary and binary)

Table 21 A List of Numerical Relationship Operators

Operator	Description
lt, <	Strictly less than
le, <=	Less than or equal to
eq, =	Equal to
ne, <>	Not equal to
ge, >=	Greater than or equal to
gt, >	Strictly greater than

Table 22 A List of Logical Operators

Operator	Description
not	Not
And	And
Or	Inclusive or
Xor	Exclusive or

Table 23 The Truth Table Generated by the Logical Operators

Operands		Results			
A	b	a and b	a or b	a xor b	not a
0	0	0	0	0	1
0	non-zero	0	1	1	1
Non-zero	0	0	1	1	0
Non-zero	non-zero	1	1	0	0

Table 24 The Operator Precedence Order in case of Mixed Logical Conditions

Operation	Operator
Exponentiation	**
Numerical Operators	
Multiplication, Division	*, /
Unary operators - Plus, Minus	+, -
Binary operators - Addition, Subtraction	+, -
Numerical Relationship Operators	<, <=, =, <>, >=, >
Logical Operators	
Not	not
And	and
Or, xor	or, xor

The functions of the logical operators are expressed in Table 23. For the mixed logical conditions, the default operator precedence order used by GAMS in the absence of parenthesis is shown in Table 24 in decreasing order. For the formulation of equations, variables can appear on the left or right-hand side of an equation or on both sides. The system can automatically convert the equation to its standard form (variables on the left, no duplicate appearances) before calling the GAMS solver. For the convenience of input, the system also provides several special notations, such as summation (sum) and product (prod), minimum value (smin), maximum value (smax).

E-3. Functions Predefined in the System

There are two types of functions based on the type of argument: exogenous or endogenous. For exogenous arguments, the arguments are known, and examples are parameters and variable attributes. The expression is evaluated once when the model is set up. All functions except the random distribution functions, uniform and normal, are allowed. With endogenous arguments, the arguments are variables, and are, therefore, unknown. The function will be evaluated many times at intermediate points while the model is being solved. The occurrence of any function with endogenous arguments implies that the model is not linear and the use of the functions of "uniform" and "normal" are forbidden in an equation definition. Some built-in functions are listed in Table 25.

E-4. Scaling Option for Variables and Equations

To facilitate the translation between a natural model (no scaling) to a well scaled model, GAMS introduces the concept of a scale factor for variables and equations with a scaling option.

This feature is incorporated in the interactive on-line optimization system to provide a well-scaled optimization problem for GAMS to solve. To use the scaling option in the interactive on-line optimization, the user must highlight the scaling option in the variable declaration and the equations declaration windows. Then, the user must enter the values of the scale factors for the variables and equations that need to be scaled. The following describes how the scale factor is incorporated in the GAMS program and how to determine the value of a scale factor.

The scale factor on a variable V^s is used to relate the variable as seen by user (in natural model) V^u to the variable as seen by the optimization algorithm (in well scaled model) V^a as follows:

$$V^u = V^a \ V^s$$

This means that the scaled variable V^a will become around 1 if the scale factor V^s is chosen to represent the order of magnitude of the user variable V^u.

If the approximate expected value for a variable in the model is known, then the magnitude of this variable value is used as the scale factor of the variable. The scale factor can be specified by users through the Measured or Unmeasured Variables window. If the approximate expected values for some of the variables in the model are not available, these values can be found in the column list of the corresponding GAMS output file. The scale factor will not change the values of variables in the solution seen by users. GAMS uses the scale factor to scale variables and transfer the model into a well scaled model for optimization algorithm. When the optimal solution is found, GAMS will rescale the variables and transfer them back to user's notation. The effect of scal
ing can only be viewed in the Column and Equation lists of the GAMS output files.

The scale factor for an equation is dependent on the order of magnitude of the equation coefficients. It is slightly different from the determination of scale factor for a variable that is dependent on the magnitude of the variable. An equation usually contains several terms, and it has several coefficients that may not be in the same order.

If the equation is linear, the coefficients of this equation is known. If the equation is nonlinear, then the equation is linearized first using the initial values. However, the linearized coefficients must be obtained from the equation list. Users can obtain the values of the linearized equation coefficients for nonlinear constraints from the equation list of the corresponding GAMS output file. To appropriately assign the scale factor for an equation, users need to carefully select the value of the scale factor based on the coefficients shown in equation list of the GAMS output file so that all coefficients will be in the range of 0.01 to 100 after scaling.

The column (variables) and equation lists are very important for nonlinear problems when scaling the variables and equations. It provides initial values of all variables and linearized constraint coefficients, which can be used to determine the scale factors for both variables and equations. It is suggested that the user turn off the scaling option for both variables and equations before GAMS is initiated.

Table 25 A List of Functions Predefined in the On-line Optimization System

Function	Description	Classification	Exogenous Classification	Endogenous model type
Abs	Absolute value	Non-smooth	Legal	DNLP
Arctan	Arctangent	Smooth	Legal	NLP
Ceil	Ceiling	Smooth	Legal	Illegal
Cos	Cosine	Discontinuous	Legal	NLP
Errorf	Error function	Smooth	Legal	NLP
Exp	Exponential	Smooth	Legal	NLP
Floor	Floor	Discontinuous	Legal	Illegal
Log	Natural log	Smooth	Legal	NLP
Log10	Common log	Smooth	Legal	NLP
Mapval	Mapping function	Discontinuous	Legal	Illegal
Max	Largest value	Non-smooth	Legal	DNLP
Min	Smallest value	Non-smooth	Legal	DNLP
Mod	Remainder	Discontinuous	Legal	Illegal
Normal	Normal random	Illegal	Illegal	Illegal
Power	Integer power	Smooth	Legal	NLP
Round	Rounding	Discontinuous	Legal	Illegal
Sign	Sign	Discontinuous	Legal	Illegal
Sin	Sine	Smooth	Legal	NLP
Sqr	Square	Smooth	Legal	NLP
Sqrt	Square root	Smooth	Legal	NLP
Trunc	Truncation	Discontinuous	Legal	Illegal
Uniform	Uniform random	Illegal	Illegal	Illegal

After the program ends, if the solution is correct and there was no difficulty in searching for an optimal solution, then the scaling option is not necessary. If the solution is not correct or some difficulty was encountered while searching for an optimal solution, then the scaling option must be incorporated in the program. In this case, users may instruct the system to include the column and equation lists in the output file. To do this, the user must change the default setting for the output files in window 12, the Output File Format Specification window. This will run the optimization program without the scaling option. Based on the values of variables in column list without scaling, users can decide the values of scale factors for variables, enter them in the

Measured Variables and Unmeasured variables windows, and highlight the icon "Include Scaling Option for variables" to scale the variables first. After the system executes the program, a new equation list, which incorporates the scale information of variables, is generated and can be used for equation scaling. Based on the linearized coefficients in this new equation list, users can determine the scale factors for the equations and enter them in the Equality Constraints and Inequality Constraints windows. Also, users must highlight the icon "Include Scaling Option for Equations" to add the Scaling Option in the programs.

E-5. Error Reporting

During compiling, executing, and solving the optimization problem, GAMS checks the input source code for program syntax, rearranges the information in the source code, and solves the optimization problem. At every step, GAMS records any error encountered and reports it in the GAMS output file. The following describes error reporting during solving the optimization problems.

Compilation Errors

The first type of error is a compilation error. When the GAMS compiler encounters an error in the input file, it inserts a coded error message inside the echo print on the line immediately following the scene of the offense. The message includes a $-symbol and an error number printed below the offending symbol (usually to the right). This error number is printed on a separate line starting with four asterisks (****). If more than one error occurs on a line, the $-signs may be suppressed and the error number is squeezed. GAMS programs are generated by the system, and no serious compilation errors are expected to appear. The most common error will be a spelling error, i.e., the variables defined in the equations may be mistyped and mismatch while declaring the variables. This will result in "variable undefined error". GAMS will not list more than 10 errors on any single line. At the end of the echo print, a list of all error numbers encountered, together with a description of the probable cause of each error, will be printed. The error messages are self-explanatory and will not be listed here. Checking the first error is recommended because it has the highest priority.

Execution Errors

The second type of error is an execution error. Execution errors are usually caused by illegal arithmetic operations such as division by zero or taking the log of a negative number. GAMS prints a message on the output file with the line number of the offending statement and continues execution. A GAMS program should never abort with an unintelligible message from the computer's operating system if an invalid operation is attempted. GAMS has rigorously defined an extended algebra that contains all operations including illegal ones. The model library problem [CRAZY] contains all non-standard operations and should be executed to study its exceptions. GAMS arithmetic is defined over the closed interval [-INF, INF] and contains values EPS (small but not zero), NA (not available), and UNDF (the result of an illegal operation). The results of illegal operations are propagated through the entire system and can be displayed with standard display statements. The model cannot be solved if errors have been detected previously.

Solve Errors

The last type of error is a solve error. The execution of a solve statement can trigger additional errors called MATRIX errors, which report on problems encountered during transformation of the model into a format required by the solver. Problems are most often caused by illegal or inconsistent bounds, or an extended range value being used as a matrix coefficient. Some solve statement require the evaluation of nonlinear functions and the computation of derivatives. Since these calculations are not carried out by the system but by other subsystems not under its direct control, errors associated with these calculations are reported in the solution report.

If the solver returns an intermediate solution because of evaluation errors, then a solution will still be attempted. The only fatal error in the system that can be caused by a solver program is the failure to return any solution at all. If this happens as mentioned above, all possible information is listed on the GAMS output file, but the solution will not be given.

XII. Acknowledgments

We gratefully acknowledge the Gulf Coast Hazardous Substance Research Center and the Environmental Protection Agency for support of this work. Also, the assistance of Ms. Gayathri Srinivasan, Mr. Tai Lee, Mr. Huitao Liu, and Ms. Qing Chen in Visual Basic programming was invaluable in developing the program.

XIII. References

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Appendix A

CONSTRAINT EQUATIONS FOR ANILINE PROCESS

In this section, the constraint equations are listed for each of the units in the aniline process shown in Figure 8. The material and energy balances as well as the reaction rate equations for the reactor are shown in Table 26. The material and energy balances as well as heat transfer equations for the heat exchangers are shown in Tables 27 through 32. In all of the heat exchangers, Q_{loss} is assumed to be zero. The material and energy balance equations for the distillation columns are shown in Tables 33 through 35. Tables 36 through 42 give the material and energy balances for the three-phase separator, the mixer, the splitter, the compressor and the pumps in the process. The material balance inequalities are shown in Table 43

Table 26. The Process Constraint Equations for the Reactor (CRV-100)

Material Balances	
Overall	$f_{09} = f_{09}^{(H_2)} + f_{09}^{(N_2)} + f_{09}^{(NH_3)} + f_{09}^{(H_2O)} + f_{09}^{(PH)} + f_{09}^{(AN)} + f_{09}^{(DPA)}$ $f_{10} = f_{10}^{(H_2)} + f_{10}^{(N_2)} + f_{10}^{(NH_3)} + f_{10}^{(H_2O)} + f_{10}^{(PH)} + f_{10}^{(AN)} + f_{10}^{(DPA)}$ $feedconc = \sum_i feed\_i \quad effconc = \sum_i eff\_i$ $i = H_2, N_2, NH_3, H_2O, PH, AN, DPA$
Species	H_2: $f_{10}^{(H_2)} - f_{09}^{(H_2)} - 1.5 * conv2 * f_{09}^{(NH_3)} = 0$ N_2: $f_{10}^{(N_2)} - f_{09}^{(N_2)} - 0.5 * conv2 * f_{09}^{(NH_3)} = 0$ NH_3: $f_{10}^{(NH_3)} - (1 - conv2) f_{09}^{(NH_3)} - 0.995 * conv1 * f_{09}^{(PH)} = 0$ H_2O: $f_{10}^{(H_2O)} - f_{09}^{(H_2O)} - conv1 * f_{09}^{(PH)} = 0$ PH: $f_{10}^{(PH)} - (1 - conv1) * f_{09}^{(PH)} = 0$ AN: $f_{10}^{(AN)} - f_{09}^{(AN)} - 0.99 * conv1 * f_{09}^{(PH)} = 0$ DPA: $f_{10}^{(DPA)} - f_{09}^{(DPA)} - 0.05 * conv1 * f_{09}^{(PH)} = 0$ $feed\_i = \frac{1000 * f_{09}^{(i)} * density_{(i)}}{f_{09} * MW_{(i)}} \quad eff\_i = \frac{1000 * f_{10}^{(i)} * density_{(i)}}{f_{10} * MW_{(i)}}$ $i = H_2, N_2, NH_3, H_2O, PH, AN, DPA$
Energy Balances	
Overall	$\sum_i f_{10}^{(i)} h_{10}^{(i)} - \sum_i f_{09}^{(i)} h_{09}^{(i)} + Q_{loss} = 0$
Enthalpy Function	$h_k^{(i)}(T) = a_1^{(i)} T + a_2^{(i)} T^2 + a_3^{(i)} T^3 + a_4^{(i)} T^4$ $i = H_2, N_2, NH_3, H_2O, PH, AN, DPA; \quad k = 10,11$ s09: all chemicals use gaseous enthalpy coefficients s10: all chemicals use gaseous enthalpy coefficients

Table 27. The Process Constraint Equations for the Cross Heat Exchanger (E-100)

Material Balances	
Overall	$(f_{08}^{(H_2)} + f_{08}^{(N_2)} + f_{08}^{(NH_3)} + f_{08}^{(H_2O)} + f_{08}^{(PH)} + f_{08}^{(AN)} + f_{08}^{(DPA)}) -$ $(f_{07}^{(H_2)} + f_{07}^{(N_2)} + f_{07}^{(NH_3)} + f_{07}^{(H_2O)} + f_{07}^{(PH)} + f_{07}^{(AN)} + f_{07}^{(DPA)}) = 0$ $(f_{11}^{(H_2)} + f_{11}^{(N_2)} + f_{11}^{(NH_3)} + f_{11}^{(H_2O)} + f_{11}^{(PH)} + f_{11}^{(AN)} + f_{11}^{(DPA)}) -$ $(f_{10}^{(H_2)} + f_{10}^{(N_2)} + f_{10}^{(NH_3)} + f_{10}^{(H_2O)} + f_{10}^{(PH)} + f_{10}^{(AN)} + f_{10}^{(DPA)}) = 0$
Species	H_2: $f_{08}^{(H_2)} - f_{07}^{(H_2)} = 0$, $f_{11}^{(H_2)} - f_{10}^{(H_2)} = 0$ N_2: $f_{08}^{(N_2)} - f_{07}^{(N_2)} = 0$, $f_{11}^{(N_2)} - f_{10}^{(N_2)} = 0$ NH_3: $f_{08}^{(NH_3)} - f_{07}^{(NH_3)} = 0$, $f_{11}^{(NH_3)} - f_{10}^{(NH_3)} = 0$ H_2O: $f_{08}^{(H_2O)} - f_{07}^{(H_2O)} = 0$, $f_{11}^{(H_2O)} - f_{10}^{(H_2O)} = 0$ PH: $f_{08}^{(PH)} - f_{07}^{(PH)} = 0$, $f_{11}^{(PH)} - f_{10}^{(PH)} = 0$ AN: $f_{08}^{(AN)} - f_{07}^{(AN)} = 0$, $f_{11}^{(AN)} - f_{10}^{(AN)} = 0$ DPA: $f_{08}^{(DPA)} - f_{07}^{(DPA)} = 0$, $f_{11}^{(DPA)} - f_{10}^{(DPA)} = 0$
Energy Balances	
Overall	$(\sum_i f_{10}^{(i)} h_{10}^{(i)} - \sum_i f_{11}^{(i)} h_{11}^{(i)}) - (\sum_i f_{08}^{(i)} h_{08}^{(i)} - \sum_i f_{07}^{(i)} h_{07}^{(i)}) + Q_{loss} = 0$ where $h_k^{(i)}(T) = a_1^{(i)} T + a_2^{(i)} T^2 + a_3^{(i)} T^3 + a_4^{(i)} T^4$ $i = H_2, N_2, NH_3, H_2O, PH, AN, DPA$; $k = 07,08,10,11$ s07: H_2, N_2, NH_3 and H_2O use gaseous enthalpy coefficients PH, AN and DPA use liquid enthalpy coefficients s08: all chemicals use gaseous enthalpy coefficients s10: all chemicals use gaseous enthalpy coefficients s11: H_2, N_2, NH_3 and H_2O use gaseous enthalpy coefficients PH, AN and DPA use liquid enthalpy coefficients
Heat Transfer	$Q_{E-100} - U_{E-100} A_{E-100} \Delta T_{LM} = 0$ $\Delta T_{LM} = \frac{(T_{10} - T_{08}) - (T_{11} - T_{07})}{\ln((T_{10} - T_{08}) / (T_{11} - T_{07}))}$

Table 28. The Process Constraint Equations for the Heater (E-101)

Material Balances	
Overall	$(f_{09}^{(H_2)} + f_{09}^{(N_2)} + f_{09}^{(NH_3)} + f_{09}^{(H_2O)} + f_{09}^{(PH)} + f_{09}^{(AN)} + f_{09}^{(DPA)}) -$ $(f_{08}^{(H_2)} + f_{08}^{(N_2)} + f_{08}^{(NH_3)} + f_{08}^{(H_2O)} + f_{08}^{(PH)} + f_{08}^{(AN)} + f_{08}^{(DPA)}) = 0$
Species	H_2: $f_{09}^{(H_2)} - f_{08}^{(H_2)} = 0$ N_2: $f_{09}^{(N_2)} - f_{08}^{(N_2)} = 0$ NH_3: $f_{09}^{(NH_3)} - f_{08}^{(NH_3)} = 0$ H_2O: $f_{09}^{(H_2O)} - f_{08}^{(H_2O)} = 0$ PH: $f_{09}^{(PH)} - f_{08}^{(PH)} = 0$ AN: $f_{09}^{(AN)} - f_{08}^{(AN)} = 0$ DPA: $f_{09}^{(DPA)} - f_{08}^{(DPA)} = 0$
Energy Balances	
Overall	$\sum_i f_{09}^{(i)} h_{09}^{(i)} - \sum_i f_{08}^{(i)} h_{08}^{(i)} - Q_{E-101} + Q_{loss} = 0$ where $h_k^{(i)}(T) = a_1^{(i)} T + a_2^{(i)} T^2 + a_3^{(i)} T^3 + a_4^{(i)} T^4$ $i = H_2, N_2, NH_3, H_2O, PH, AN, DPA;$ $k = 08,09$ s08: all chemicals use gaseous enthalpy coefficients s09: all chemicals use gaseous enthalpy coefficients

Table 29. The Process Constraint Equations for the Reactor Product Cooler (E-102)

Material Balances	
Overall	$(f_{12}^{(H_2)} + f_{12}^{(N_2)} + f_{12}^{(NH_3)} + f_{12}^{(H_2O)} + f_{12}^{(PH)} + f_{12}^{(AN)} + f_{12}^{(DPA)}) -$ $(f_{11}^{(H_2)} + f_{11}^{(N_2)} + f_{11}^{(NH_3)} + f_{11}^{(H_2O)} + f_{11}^{(PH)} + f_{11}^{(AN)} + f_{11}^{(DPA)}) = 0$ $f_{CW2} - f_{CW1} = 0$ where CW = cooling water
Species	H_2: $f_{12}^{(H_2)} - f_{11}^{(H_2)} = 0$ N_2: $f_{12}^{(N_2)} - f_{11}^{(N_2)} = 0$ NH_3: $f_{12}^{(NH_3)} - f_{11}^{(NH_3)} = 0$ H_2O: $f_{12}^{(H_2O)} - f_{11}^{(H_2O)} = 0$ $f_{CW2} - f_{CW1} = 0$ PH: $f_{12}^{(PH)} - f_{11}^{(PH)} = 0$ AN: $f_{12}^{(AN)} - f_{11}^{(AN)} = 0$ DPA: $f_{12}^{(DPA)} - f_{11}^{(DPA)} = 0$
Energy Balances	
Overall	$\sum_i f_{CW2} h_{CW2} - \sum_i f_{CW1} h_{CW1} - Q_{E-102} + Q_{loss} = 0$ where $h_{CW(j)}(T) = a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4$ a_1 through a_4 are for liquid water; j = 1,2 $\sum_i f_{11}^{(i)} * h_{11}^{(i)} - H_{12} - Q_{E-102} = 0$ where $h_{11}^{(i)}(T) = a_1^{(i)} T + a_2^{(i)} T^2 + a_3^{(i)} T^3 + a_4^{(i)} T^4$ $i = H_2, N_2, NH_3, H_2O, PH, AN, DPA$ s11: H_2, N_2, NH_3 and H_2O use gaseous enthalpy coefficients PH, AN and DPA use liquid enthalpy coefficients
Heat Transfer	$Q_{E-102} - U_{E-102} A_{E-102} \Delta T_{LM} = 0$ $\Delta T_{LM} = \frac{(T_{11} - T_{CW2}) - (T_{12} - T_{CW1})}{\ln((T_{11} - T_{CW2})/(T_{12} - T_{CW1}))}$

Table 30. The Process Constraint Equations for the Drying Column Cooler (E-103)

Material Balances	
Overall	$(f_{20}^{(NH_3)} + f_{20}^{(H_2O)} + f_{20}^{(PH)} + f_{20}^{(AN)}) - (f_{19}^{(NH_3)} + f_{19}^{(H_2O)} + f_{19}^{(PH)} + f_{19}^{(AN)}) = 0$ $f_{CW4} - f_{CW3} = 0$ where CW = cooling water
Species	NH_3: $f_{20}^{(NH_3)} - f_{19}^{(NH_3)} = 0$ H_2O: $f_{20}^{(H_2O)} - f_{19}^{(H_2O)} = 0$ $f_{CW4} - f_{CW3} = 0$ PH: $f_{20}^{(PH)} - f_{19}^{(PH)} = 0$ AN: $f_{20}^{(AN)} - f_{19}^{(AN)} = 0$
Energy Balances	
Overall	$\sum_i f_{CW4} h_{CW4} - \sum_i f_{CW3} h_{CW3} - Q_{E-103} + Q_{loss} = 0$ where $h_{CW(j)}(T) = a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4$ a_1 through a_4 are for liquid water; $j = 3,4$ $\sum_i f_{19}^{(i)} h_{19}^{(i)} - H_{20} - Q_{E-103} = 0$ where $h_{19}^{(i)}(T) = a_1^{(i)} T + a_2^{(i)} T^2 + a_3^{(i)} T^3 + a_4^{(i)} T^4$ $i = NH_3, H_2O, PH, AN$ s19: all chemicals use gaseous enthalpy coefficients
Heat Transfer	$Q_{E-103} - U_{E-103} A_{E-103} \Delta T_{LM} = 0$ $\Delta T_{LM} = \frac{(T_{19} - T_{CW4}) - (T_{20} - T_{CW3})}{\ln((T_{19} - T_{CW4})/(T_{20} - T_{CW3}))}$

Table 31. The Constraint Equations for the Aniline Product Cooler (E-104)

Material Balances	
Overall	$(f_{28}^{(H_2O)} + f_{28}^{(PH)} + f_{28}^{(AN)}) - (f_{27}^{(H_2O)} + f_{27}^{(PH)} + f_{27}^{(AN)}) = 0$ $f_{CW6} - f_{CW5} = 0$ where CW = cooling water
Species	H_2O: $f_{28}^{(H_2O)} - f_{27}^{(H_2O)} = 0$ $f_{CW6} - f_{CW5} = 0$ PH: $f_{28}^{(PH)} - f_{27}^{(PH)} = 0$ AN: $f_{28}^{(AN)} - f_{27}^{(AN)} = 0$
Energy Balances	
Overall	$\sum_i f_{CW6} h_{CW6} - \sum_i f_{CW5} h_{CW5} - Q_{E-104} + Q_{loss} = 0$ where $h_{CW(j)}(T) = a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4$ a_1 through a_4 are for water; $j = 5,6$ $\sum_i f_{27}^{(i)} h_{27}^{(i)} - H_{28} - Q_{E-104} = 0$ where $h_{27}^{(i)}(T) = a_1^{(i)} T + a_2^{(i)} T^2 + a_3^{(i)} T^3 + a_4^{(i)} T^4$ $i = H_2O, PH, AN$ s27: all chemicals use liquid enthalpy coefficients
Heat Transfer	$Q_{E-104} - U_{E-104} A_{E-104} \Delta T_{LM} = 0$ $\Delta T_{LM} = \frac{(T_{27} - T_{CW6}) - (T_{28} - T_{CW5})}{\ln((T_{27} - T_{CW6})/(T_{28} - T_{CW5}))}$

Table 32. The Constraint Equations for the DPA Product Cooler (E-105)

Material Balances	
Overall	$(f_{33}^{(PH)} + f_{33}^{(DPA)}) - (f_{32}^{(PH)} + f_{32}^{(DPA)}) = 0$ $f_{CW8} - f_{CW7} = 0$ where CW = cooling water
Species	H_2O: $f_{CW8} - f_{CW7} = 0$ PH: $f_{33}^{(PH)} - f_{32}^{(PH)} = 0$ DPA: $f_{33}^{(DPA)} - f_{32}^{(DPA)} = 0$
Energy Balances	
Overall	$\sum_i f_{CW8} h_{CW8} - \sum_i f_{CW7} h_{CW7} - Q_{E-105} + Q_{loss} = 0$ where $h_{CW(j)}(T) = a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4$ a_1 through a_4 are for water; $j = 7,8$ $\sum_i f_{32}^{(i)} h_{32}^{(i)} - H_{33} - Q_{E-105} = 0$ where $h_{32}^{(i)}(T) = a_1^{(i)} T + a_2^{(i)} T^2 + a_3^{(i)} T^3 + a_4^{(i)} T^4$ $i = PH, DPA$ s32: all chemicals use liquid enthalpy coefficients
Heat Transfer	$Q_{E-105} - U_{E-105} A_{E-105} \Delta T_{LM} = 0$ $\Delta T_{LM} = \frac{(T_{32} - T_{CW7}) - (T_{33} - T_{CW8})}{\ln((T_{32} - T_{CW7})/(T_{33} - T_{CW8}))}$

Table 33. The Constraint Equations for the Absorption Tower (T-100)

Material Balances	
Overall	$(f_{13}^{(H_2)} + f_{13}^{(N_2)} + f_{13}^{(NH_3)} + f_{13}^{(H_2O)}) +$ $(f_{18}^{(NH_3)} + f_{18}^{(H_2O)} + f_{18}^{(PH)} + f_{18}^{(AN)} + f_{18}^{(DPA)}) -$ $(f_{12}^{(H_2)} + f_{12}^{(N_2)} + f_{12}^{(NH_3)} + f_{12}^{(H_2O)} + f_{12}^{(PH)} + f_{12}^{(AN)} + f_{12}^{(DPA)}) = 0$
Species	H_2: $f_{13}^{(H_2)} - f_{12}^{(H_2)} = 0$ N_2: $f_{13}^{(N_2)} - f_{12}^{(N_2)} = 0$ NH_3: $f_{13}^{(NH_3)} - 0.999 f_{12}^{(NH_3)} = 0$ $f_{18}^{(NH_3)} - 0.001 f_{12}^{(NH_3)} = 0$ H_2O: $f_{13}^{(H_2O)} - 0.10 f_{12}^{(H_2O)} = 0$ $f_{18}^{(H_2O)} - 0.90 f_{12}^{(H_2O)} = 0$ PH: $f_{18}^{(PH)} - f_{12}^{(PH)} = 0$ AN: $f_{18}^{(AN)} - f_{12}^{(AN)} = 0$ DPA: $f_{18}^{(DPA)} - f_{12}^{(DPA)} = 0$
Energy Balances	
Enthalpy Function	$h_k^{(i)}(T) = a_1^{(i)}T + a_2^{(i)}T^2 + a_3^{(i)}T^3 + a_4^{(i)}T^4$ $i = H_2, N_2, NH_3, H_2O, PH, AN, DPA$; $k = 13,18$ s13: all chemicals use gaseous enthalpy coefficients s18: all chemicals use gaseous enthalpy coefficients

Table 34. The Constraint Equations for the Drying Column (T-101)

Material Balances	
Overall	$(f_{19}^{(NH_3)} + f_{19}^{(H_2O)} + f_{19}^{(PH)} + f_{19}^{(AN)}) + (f_{25}^{(H_2O)} + f_{25}^{(PH)} + f_{25}^{(AN)} + f_{25}^{(DPA)}) -$ $(f_{18}^{(NH_3)} + f_{18}^{(H_2O)} + f_{18}^{(PH)} + f_{18}^{(AN)} + f_{18}^{(DPA)}) = 0$
Species	NH_3: $f_{19}^{(NH_3)} - (f_{18}^{(NH_3)} + f_{23}^{(NH_3)}) = 0$ H_2O: $f_{19}^{(H_2O)} - 0.9999(f_{18}^{(H_2O)} + f_{23}^{(H_2O)}) = 0$ $f_{25}^{(H_2O)} - 0.0001(f_{18}^{(H_2O)} + f_{23}^{(H_2O)}) = 0$ PH: $f_{19}^{(PH)} - 0.06(f_{18}^{(PH)} + f_{23}^{(PH)}) = 0$ $f_{25}^{(PH)} - 0.94(f_{18}^{(PH)} + f_{23}^{(PH)}) = 0$ AN: $f_{19}^{(AN)} - 0.05(f_{18}^{(AN)} + f_{23}^{(AN)}) = 0$ $f_{25}^{(AN)} - 0.95(f_{18}^{(AN)} + f_{23}^{(AN)}) = 0$ DPA: $f_{25}^{(DPA)} - f_{18}^{(DPA)} = 0$
Energy Balances	
Enthalpy Function	$h_k^{(i)}(T) = a_1^{(i)}T + a_2^{(i)}T^2 + a_3^{(i)}T^3 + a_4^{(i)}T^4$ $i = NH_3, H_2O, PH, AN, DPA;$ $k = 18,19,25$ s18: all chemicals use liquid enthalpy coefficients s19: all chemicals use gaseous enthalpy coefficients s25: all chemicals use liquid enthalpy coefficients

Table 35. The Constraint Equations for the Product Column (T-102)

Material Balances	
Overall	$(f_{26}^{(H_2O)} + f_{26}^{(PH)} + f_{26}^{(AN)}) + (f_{29}^{(PH)} + f_{29}^{(AN)} + f_{29}^{(DPA)}) +$ $(f_{32}^{(PH)} + f_{32}^{(AN)} + f_{32}^{(DPA)}) - (f_{25}^{(H_2O)} + f_{25}^{(PH)} + f_{25}^{(AN)} + f_{25}^{(DPA)}) = 0$
Species	H_2O: $f_{26}^{(H_2O)} - 0.10 f_{25}^{(H_2O)} = 0$ PH: $f_{26}^{(PH)} - 0.195 f_{25}^{(PH)} = 0$ $f_{29}^{(PH)} - 0.80 f_{25}^{(PH)} = 0$ $f_{32}^{(PH)} - 0.005 f_{25}^{(PH)} = 0$ AN: $f_{26}^{(AN)} - 0.923 f_{25}^{(AN)} = 0$ $f_{29}^{(AN)} - 0.077 f_{25}^{(AN)} = 0$ $f_{32}^{(AN)} - 0.000246 f_{25}^{(AN)} = 0$ DPA: $f_{29}^{(DPA)} - 0.046 f_{25}^{(DPA)} = 0$ $f_{32}^{(DPA)} - 0.954 f_{25}^{(DPA)} = 0$
Energy Balances	
Enthalpy Function	$h_k^{(i)}(T) = a_1^{(i)} T + a_2^{(i)} T^2 + a_3^{(i)} T^3 + a_4^{(i)} T^4$ $i = H_2O, PH, AN, DPA;$ $k = 25,26,29,32$ s25: all chemicals use liquid enthalpy coefficients s26: all chemicals use liquid enthalpy coefficients s29: all chemicals use liquid enthalpy coefficients s32: all chemicals use liquid enthalpy coefficients

Table 36. The Process Constraint Equations for the Three-Phase Separator (V-100)

Material Balances	
Overall	$(f_{21}^{(NH_3)} + f_{21}^{(H_2O)} + f_{21}^{(PH)} + f_{21}^{(AN)}) + (f_{24}^{(NH_3)} + f_{24}^{(H_2O)} + f_{24}^{(PH)} + f_{24}^{(AN)}) -$ $(f_{20}^{(NH_3)} + f_{20}^{(H_2O)} + f_{20}^{(PH)} + f_{20}^{(AN)}) = 0$
Species	NH_3: $f_{21}^{(NH_3)} - 0.07 f_{20}^{(NH_3)} = 0$ $f_{24}^{(NH_3)} - 0.93 f_{20}^{(NH_3)} = 0$ H_2O: $f_{21}^{(H_2O)} - 0.03 f_{20}^{(H_2O)} = 0$ $f_{24}^{(H_2O)} - 0.97 f_{20}^{(H_2O)} = 0$ PH: $f_{21}^{(PH)} - 0.305 f_{20}^{(PH)} = 0$ $f_{24}^{(PH)} - 0.695 f_{20}^{(PH)} = 0$ AN: $f_{21}^{(AN)} - 0.86 f_{20}^{(AN)} = 0$ $f_{24}^{(AN)} - 0.14 f_{20}^{(AN)} = 0$
Energy Balances	
Enthalpy Function	$h_k^{(i)}(T) = a_1^{(i)}T + a_2^{(i)}T^2 + a_3^{(i)}T^3 + a_4^{(i)}T^4$ $i = NH_3, H_2O, PH, AN;$ $k = 21,24$ s21: all chemicals use liquid enthalpy coefficients s24: all chemicals use liquid enthalpy coefficients

Table 37. The Constraint Equations for the Mixer (MIX-102)

Material Balances	
Overall	$(f_{07}^{(H_2)} + f_{07}^{(N_2)} + f_{07}^{(NH_3)} + f_{07}^{(H_2O)} + f_{07}^{(PH)} + f_{07}^{(AN)} + f_{07}^{(DPA)}) - f_{03}^{(NH3)} - f_{04}^{(PH)} - (f_{16}^{(H_2)} + f_{16}^{(N_2)} + f_{16}^{(NH_3)} + f_{16}^{(H_2O)}) - (f_{31}^{(PH)} + f_{31}^{(AN)} + f_{31}^{(DPA)}) = 0$
Species	H_2: $f_{07}^{(H_2)} - f_{16}^{(H_2)} = 0$ N_2: $f_{07}^{(N_2)} - f_{16}^{(N_2)} = 0$ NH_3: $f_{07}^{(NH_3)} - f_{03}^{(NH_3)} - f_{16}^{(NH3)} = 0$ H_2O: $f_{07}^{(H_2O)} - f_{16}^{(H_2O)} = 0$ PH: $f_{07}^{(PH)} - f_{03}^{(PH)} - f_{31}^{(PH)} = 0$ AN: $f_{07}^{(AN)} - f_{31}^{(AN)} = 0$ DPA: $f_{07}^{(DPA)} - f_{31}^{(DPA)} = 0$
Energy Balances	
Overall	$\sum_i f_{07}^{(i)} h_{07}^{(i)} - f_{03}^{(NH_3)} h_{03}^{(NH_3)} - f_{04}^{(PH)} h_{04}^{(PH)} - \sum_i f_{31}^{(i)} h_{31}^{(i)} + Q_{loss} = 0$
Enthalpy Function	$h_k^{(i)}(T) = a_1^{(i)} T + a_2^{(i)} T^2 + a_3^{(i)} T^3 + a_4^{(i)} T^4$ $i = H_2, N_2, NH_3, H_2O, PH, AN, DPA$; $k = 03,04,07,16,31$ s03: NH3 uses liquid enthalpy coefficients s04: PH uses liquid enthalpy coefficients s07: H2, N2, NH3 and H2O use gaseous enthalpy coefficients PH, AN and DPA use liquid enthalpy coefficients s16: all chemicals use gaseous enthalpy coefficients s31: all chemicals use liquid enthalpy coefficients

Table 38. The Constraint Equations for the Splitter (TEE-100)

Material Balances	
Overall	$(f_{14}^{(H_2)} + f_{14}^{(N_2)} + f_{14}^{(NH_3)} + f_{14}^{(H_2O)}) + (f_{17}^{(H_2)} + f_{17}^{(N_2)} + f_{17}^{(NH_3)} + f_{17}^{(H_2O)}) -$ $(f_{13}^{(H_2)} + f_{13}^{(N_2)} + f_{13}^{(NH_3)} + f_{13}^{(H_2O)}) = 0$
Species	H_2: $f_{14}^{(H_2)} + f_{17}^{(H_2)} - f_{13}^{(H_2)} = 0$ N_2: $f_{14}^{(N_2)} + f_{17}^{(N_2)} - f_{13}^{(N_2)} = 0$ NH_3: $f_{14}^{(NH_3)} + f_{17}^{(NH_3)} - f_{13}^{(NH_3)} = 0$ H_2O: $f_{14}^{(H_2O)} + f_{17}^{(H_2O)} - f_{13}^{(H_2O)} = 0$
Energy Balances	
Overall	$H_{14} + H_{17} - \sum_i f_{13}^{(i)} h_{13}^{(i)} = 0$
Enthalpy Function	$H_{14} - 0.989 * \sum_i f_{13}^{(i)} h_{13}^{(i)} = 0$ $H_{17} - 0.011 * \sum_i f_{13}^{(i)} h_{13}^{(i)} = 0$ $h_{13}^{(i)}(T) = a_1^{(i)} T + a_2^{(i)} T^2 + a_3^{(i)} T^3 + a_4^{(i)} T^4$ $i = H_2, N_2, NH_3, H_2O$ s13: all chemicals use gaseous enthalpy coefficients

Table 39. The Process Constraint Equations for the Compressor (K-100)

Material Balances	
Overall	$(f_{16}^{(H_2)} + f_{16}^{(N_2)} + f_{16}^{(NH_3)} + f_{16}^{(H_2O)}) - (f_{14}^{(H_2)} + f_{14}^{(N_2)} + f_{14}^{(NH_3)} + f_{14}^{(H_2O)}) = 0$
Species	H_2: $f_{16}^{(H_2)} - f_{14}^{(H_2)} = 0$ N_2: $f_{16}^{(N_2)} - f_{14}^{(N_2)} = 0$ NH_3: $f_{16}^{(NH_3)} - f_{14}^{(NH_3)} = 0$ H_2O: $f_{16}^{(H_2O)} - f_{14}^{(H_2O)} = 0$
Energy Balances	
Enthalpy Function	$h_k^{(i)}(T) = a_1^{(i)} T + a_2^{(i)} T^2 + a_3^{(i)} T^3 + a_4^{(i)} T^4$ $i = H_2, N_2, NH_3, H_2O; \quad k = 14,16$ s14: all chemicals use gaseous enthalpy coefficients s16: all chemicals use gaseous enthalpy coefficients

Table 40. The Process Constraint Equations for the Drying Column Recycle Pump (P-102)

Material Balances	
Overall	$(f_{23}^{(NH_3)} + f_{23}^{(H_2O)} + f_{23}^{(PH)} + f_{23}^{(AN)}) - (f_{21}^{(NH_3)} + f_{21}^{(H_2O)} + f_{21}^{(PH)} + f_{21}^{(AN)}) = 0$
Species	NH_3: $f_{23}^{(NH_3)} - f_{21}^{(NH_3)} = 0$ H_2O: $f_{23}^{(H_2O)} - f_{21}^{(H_2O)} = 0$ PH: $f_{23}^{(PH)} - f_{21}^{(PH)} = 0$ AN: $f_{23}^{(AN)} - f_{21}^{(AN)} = 0$
Energy Balances	
Enthalpy Function	$h_k^{(i)}(T) = a_1^{(i)}T + a_2^{(i)}T^2 + a_3^{(i)}T^3 + a_4^{(i)}T^4$ $i = NH_3, H_2O, PH, AN$; $k = 21,23$ s21: all chemicals use liquid enthalpy coefficients s23: all chemicals use liquid enthalpy coefficients

Table 41. The Process Constraint Equations for the Phenol Recycle Pump (P-103)

Material Balances	
Overall	$(f_{31}^{(PH)} + f_{31}^{(AN)} + f_{31}^{(DPA)}) - (f_{29}^{(PH)} + f_{29}^{(AN)} + f_{29}^{(DPA)}) = 0$
Species	PH: $f_{31}^{(PH)} - f_{29}^{(PH)} = 0$ AN: $f_{31}^{(AN)} - f_{29}^{(AN)} = 0$ DPA: $f_{31}^{(DPA)} - f_{29}^{(DPA)} = 0$
Energy Balances	
Enthalpy Function	$h_k^{(i)}(T) = a_1^{(i)}T + a_2^{(i)}T^2 + a_3^{(i)}T^3 + a_4^{(i)}T^4$ $i = PH, AN, DPA$; $k = 29,31$ s29: all chemicals use liquid enthalpy coefficients s31: all chemicals use liquid enthalpy coefficients

Table 42. The Process Constraint Equations for the Aniline Product Pump (P-104)

Material Balances	
Overall	$(f_{27}^{(H_2O)} + f_{27}^{(PH)} + f_{27}^{(AN)}) - (f_{26}^{(H_2O)} + f_{26}^{(PH)} + f_{26}^{(AN)}) = 0$
Species	H_2O: $f_{27}^{(H_2O)} - f_{26}^{(H_2O)} = 0$ PH: $f_{27}^{(PH)} - f_{26}^{(PH)} = 0$ AN: $f_{27}^{(AN)} - f_{26}^{(AN)} = 0$
Energy Balances	
Enthalpy Function	$h_k^{(i)}(T) = a_1^{(i)}T + a_2^{(i)}T^2 + a_3^{(i)}T^3 + a_4^{(i)}T^4$ $i = H_2O, PH, AN;$ $k = 26,27$ s26: all chemicals use liquid enthalpy coefficients s27: all chemicals use liquid enthalpy coefficients

Table 43. The Process Constraint Inequalities

Material Balances	
Mixed Stream	$\frac{f_{07}^{(NH_3)}}{f_{07}^{(PH)}} \geq 17$
Aniline Product	$f_{26}^{(AN)} \geq \frac{0.989(f_{26}^{(H_2O)} MW_{H_2O} + f_{26}^{(PH)} MW_{PH} + f_{26}^{(AN)} MW_{AN})}{MW_{AN}}$
Phenol Recycle	$f_{29}^{(PH)} \geq \frac{0.30(f_{29}^{(PH)} MW_{PH} + f_{29}^{(AN)} MW_{AN} + f_{29}^{(DPA)} MW_{DPA})}{MW_{PH}}$ $f_{29}^{(AN)} \geq \frac{0.65(f_{29}^{(PH)} MW_{PH} + f_{29}^{(AN)} MW_{AN} + f_{29}^{(DPA)} MW_{DPA})}{MW_{AN}}$
DPA Product	$f_{32}^{(DPA)} \geq \frac{0.945(f_{32}^{(PH)} MW_{PH} + f_{32}^{(DPA)} MW_{DPA})}{MW_{DPA}}$
Energy Balances	
E-100 Temperature Approach	$T_{10} - T_{08} \geq 75$
E-102 Temperature Approach	$T_{12} - T_{CW_1} \geq 60$
E-103 Temperature Approach	$T_{20} - T_{CW_3} \geq 30$
E-104 Temperature Approach	$T_{27} - T_{CW_5} \geq 10$
E-105 Temperature Approach	$T_{33} - T_{CW_7} \geq 50$

Appendix B

Full Output File for Economic Optimization (Profit Maximization) of the Aniline Process


```
  2
  5
  6  SCALARS
  7  h2  / 2 /
  8  n2  / 28 /
  9  nh3  / 17 /
 10  h2o  / 18 /
 11  ph  / 94 /
 12  an  / 93 /
 13  dpa  / 169 /
 14  ;
 15
 16  SCALARS
 17  areaE100  / 6900 /
 18  areaE102  / 1725 /
 19  areaE103  / 760 /
 20  areaE104  / 310 /
 21  areaE105  / 2 /
 22  ;
 23  SCALARS
 24  dens_h2  / 0.0349 /
 25  dens_n2  / 0.019 /
 26  dens_nh3  / 2.1117 /
 27  dens_h2o  / 0.3209 /
 28  dens_ph  / 39.7521 /
 29  dens_an  / 37.518 /
 30  dens_dpa  / 43.608 /
 31  ;
 32  SCALARS
 33  price_nh3  / 0.0875 /
 34  price_ph  / 0.38 /
 35  price_an  / 0.49 /
 36  price_dpa  / 1.8 /
 37  ;
 38  SCALARS
 39  hfh2  / 0 /
 40  hfn2  / 0 /
 41  hfnh3  /-19733 /
 42  hfh2o  /-103955 /
 43  hfph  /-41427 /
 44  hfan  / 37343 /
 45  hfdpa  / 86844 /
 46  ;
 47
 48  * The following are the Measured Variables
 49  VARIABLES
```



```
 50  f03, f04, f07, f08, f09, f10, f11, f12,
 51  f13, f14, f16, f17, f18, f19, f20, f21,
 52  f23, f24, f25, f26, f27, f28, f29, f31,
 53  f32, f33, fCW1, fCW2, fCW3, fCW4, fCW5, fCW6,
 54  fCW7, fCW8, T03, T04, T07, T08, T09, T10,
 55  T11, T12, T13, T14, T16, T17, T18, T19,
 56  T20, T21, T23, T24, T25, T26, T27, T28,
 57  T29, T31, T32, T33, TCW1, TCW2, TCW3, TCW4,
 58  TCW5, TCW6, TCW7, TCW8;
 59
 60  VARIABLE ObjVar objective or profit function;
 61  * The following are the Unmeasured Variables
 62  VARIABLES
 63  eff_an, eff_dpa, eff_h2, eff_h2o, eff_n2, eff_nh3, eff_ph, f03nh3,
 64  f04ph, f07an, f07dpa, f07h2, f07h2o, f07n2, f07nh3, f07ph,
 65  f08an, f08dpa, f08h2, f08h2o, f08n2, f08nh3, f08ph, f09an,
 66  f09dpa, f09h2, f09h2o, f09n2, f09nh3, f09ph, f10an, f10dpa,
 67  f10h2, f10h2o, f10n2, f10nh3, f10ph, f11an, f11dpa, f11h2,
 68  f11h2o, f11n2, f11nh3, f11ph, f12an, f12dpa, f12h2, f12h2o,
 69  f12n2, f12nh3, f12ph, f13h2, f13h2o, f13n2, f13nh3, f14h2,
 70  f14h2o, f14n2, f14nh3, f16h2, f16h2o, f16n2, f16nh3, f17h2,
 71  f17h2o, f17n2, f17nh3, f18an, f18dpa, f18h2o, f18nh3, f18ph,
```

```
  72  f19an, f19h2o, f19nh3, f19ph, f20an, f20h2o, f20nh3, f20ph,
  73  f21an, f21h2o, f21nh3, f21ph, f23an, f23h2o, f23nh3, f23ph,
  74  f24an, f24h2o, f24nh3, f24ph, f25an, f25dpa, f25h2o, f25ph,
  75  f26an, f26h2o, f26ph, f27an, f27h2o, f27ph, f28an, f28h2o,
  76  f28ph, f29an, f29dpa, f29ph, f31an, f31dpa, f31ph, f32an,
  77  f32dpa, f32ph, f33an, f33dpa, f33ph, feed_an, feed_dpa, feed_h2,
  78  feed_h2o, feed_n2, feed_nh3, feed_ph, H03, H04, H07, H08,
  79  H09, H10, H11, H12, H13, H14, H16, H17,
  80  H18, H19, H20, H21, H23, H24, H25, H26,
  81  H27, H28, H29, H31, H32, H33, profit, Q100,
  82  Q101, Q102, Q103, Q104, Q105, TE100, TE102, TE103,
  83  TE104, TE105;
  84
  85  * The following are the Parameters in the Model
  86  SCALARS
  87  conv1      / 0.94948 /
  88  conv2      / 0.001 /
  89  uE100      / 51.89313 /
  90  uE102      / 54.77626 /
  91  uE103      / 71.41481 /
  92  uE104      / 71.78423 /
  93  uE105      / 80.78474 /
  94  ;
  95
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  96  VARIABLES
  97  ObjVar Objective function using ' ' algorithm;
  98
  99  SETS
 100   coeff1 /a1,a2,a3,a4/
 101   comp1 /h2, n2, nh3, h2o, ph, an, dpa/
 102   coeff2 /a1,a2,a3,a4/
 103   comp2 /nh3, h2o, ph, an, dpa/
 104   ;
 105   TABLE enth_gas(comp1,coeff1)
 106                a1          a2          a3          a4
 107  h2             6.7762      1.2745E-04  -3.1784E-08  1.2545E-11
 108  n2             6.9872     -1.9897E-04   2.2049E-07  -3.4903E-11
 109  nh3            6.5140      1.7334E-03   2.4376E-07  -6.9535E-11
 110  h2o            7.8055     -4.7750E-05   3.4883E-07  -5.0150E-11
 111  ph            -3.4274      3.1755E-02  -7.2633E-06   6.7130E-10
 112  an            -2.8491      3.3895E-02  -8.0960E-06   8.1465E-10
 113  dpa           -19.242      7.0815E-02  -1.8014E-06   1.9146E-09
 114   TABLE enth_liq(comp2,coeff2)
 115                a1          a2          a3          a4
 116  nh3           -43.507      2.2304E-01  -3.5380E-04   2.0857E-07
 117  h2o            21.986     -2.6508E-03  -5.1857E-06   5.4745E-09
 118  ph             9.2247      7.2870E-02  -6.1180E-05   2.3346E-08
 119  an            15.116       6.5655E-02  -5.7950E-05   2.3852E-08
 120  dpa            17.304      9.6945E-02  -7.2647E-05   2.4965E-08
 121
 122  EQUATIONS
 123  * The Constraints
 124  EQU1, EQU2, EQU3, EQU4, EQU5, EQU6,
 125  EQU7, EQU8, EQU9, EQU10, EQU11, EQU12,
 126  EQU13, EQU14, EQU15, EQU16, EQU17, EQU18,
 127  EQU19, EQU20, EQU21, EQU22, EQU23, EQU24,
 128  EQU25, EQU26, EQU27, EQU28, EQU29, EQU30,
 129  EQU31, EQU32, EQU33, EQU34, EQU35, EQU36,
 130  EQU37, EQU38, EQU39, EQU40, EQU41, EQU42,
 131  EQU43, EQU44, EQU45, EQU46, EQU47, EQU48,
 132  EQU49, EQU50, EQU51, EQU52, EQU53, EQU54,
 133  EQU55, EQU56, EQU57, EQU58, EQU59, EQU60,
 134  EQU61, EQU62, EQU63, EQU64, EQU65, EQU66,
 135  EQU67, EQU68, EQU69, EQU70, EQU71, EQU72,
 136  EQU73, EQU74, EQU75, EQU76, EQU77, EQU78,
 137  EQU79, EQU80, EQU81, EQU82, EQU83, EQU84,
 138  EQU85, EQU86, EQU87, EQU88, EQU89, EQU90,
 139  EQU91, EQU92, EQU93, EQU94, EQU95, EQU96,
 140  EQU97, EQU98, EQU99, EQU100, EQU101, EQU102,
 141  EQU103, EQU104, EQU105, EQU106, EQU107, EQU108,
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 142  EQU109, EQU110, EQU111, EQU112, EQU113, EQU114,
 143  EQU115, EQU116, EQU117, EQU118, EQU119, EQU120,
 144  EQU121, EQU122, EQU123, EQU124, EQU125, EQU126,
 145  EQU127, EQU128, EQU129, EQU130, EQU131, EQU132,
 146  EQU133, EQU134, EQU135, EQU136, EQU137, EQU138,
 147  EQU139, EQU140, EQU141, EQU142, EQU143, EQU144,
 148  EQU145, EQU146, EQU147, EQU148, EQU149, EQU150,
 149  EQU151, EQU152, EQU153, EQU154, EQU155, EQU156,
 150  EQU157, EQU158, EQU159, EQU160, EQU161, EQU162,
 151  EQU163, EQU164, EQU165, EQU166, EQU167, EQU168,
 152  EQU169, EQU170, EQU171, EQU172, EQU173, EQU174,
 153  EQU175, EQU176, EQU177, EQU178, EQU179, EQU180,
 154  EQU181, EQU182, EQU183, EQU184, EQU185, EQU186,
 155  EQU187, EQU188, EQU189, EQU190, EQU191, EQU192,
```

```
156  EQU193, EQU194, EQU195, EQU196, EQU197, EQU198,
157   EQU199, EQU200,
158  INEQU1, INEQU2, INEQU3, INEQU4, INEQU5, INEQU6,
159  INEQU7, INEQU8, INEQU9, INEQU10, ObjName;
160
161  ObjName..ObjVar=E=
162  profit;
163
164  EQU1..f10ph-((1-conv1)*f09ph) =e= 0;
165  EQU2..f10an-(f09an+0.985*conv1*f09ph) =e= 0;
166  EQU3..f10dpa-(f09dpa+0.005*conv1*f09ph) =e= 0;
167  EQU4..H10-H09 =e= 0;
168  EQU5..T10-T09 =e= 15;
169  EQU6..f10-(f10h2+f10n2+f10nh3+f10h2o+f10ph+f10an+f10dpa) =e= 0;
170  EQU7..f11h2-f10h2 =e= 0;
171  EQU8..f11n2-f10n2 =e= 0;
172  EQU9..f11nh3-f10nh3 =e= 0;
173  EQU10..f11h2o-f10h2o =e= 0;
174  EQU11..f11ph-f10ph =e= 0;
175  EQU12..f11an-f10an =e= 0;
176  EQU13..f11dpa-f10dpa =e= 0;
177  EQU14..TE100-(((T10-T08)-(T11-T07))/log((T10-T08)/(T11-T07))) =e= 0;
178  EQU15..Q100-areaE100*uE100*TE100/1000000 =e= 0;
179  EQU16..Q100-(H10-H11) =e= 0;
180  EQU17..f11-(f11h2+f11n2+f11nh3+f11h2o+f11ph+f11an+f11dpa) =e= 0;
181  EQU18..H11-((f11h2*(hfh2+sum(coeff1,enth_gas("h2",coeff1)*(power(T11,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
182  (f11n2*(hfn2+sum(coeff1,enth_gas("n2",coeff1)*(power(T11,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
183  (f11nh3*(hfnh3+sum(coeff1,enth_gas("nh3",coeff1)*(power(T11,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
184  (f11h2o*(hfh2o+sum(coeff1,enth_gas("h2o",coeff1)*(power(T11,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
185  (f11ph*(hfph+sum(coeff2,enth_liq("ph",coeff2)*(power(T11,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000) +
186  (f11an*(hfan+sum(coeff2,enth_liq("an",coeff2)*(power(T11,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000) +
187  (f11dpa*(hfdpa+sum(coeff2,enth_liq("dpa",coeff2)*(power(T11,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000)) =e= 0;
```



```
188  EQU19..f12h2-f11h2 =e= 0;
189  EQU20..f12n2-f11n2 =e= 0;
190  EQU21..f12nh3-f11nh3 =e= 0;
191  EQU22..f12h2o-f11h2o =e= 0;
192  EQU23..f12ph-f11ph =e= 0;
193  EQU24..f12an-f11an =e= 0;
194  EQU25..f12dpa-f11dpa =e= 0;
195  EQU26..fCW2-fCW1 =e= 0;
196  EQU27..Q102-((fCW2*(hfh2o+sum(coeff2,enth_liq("h2o",coeff2)*(power(TCW2,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000) -
197  (fCW1*(hfh2o+sum(coeff2,enth_liq("h2o",coeff2)*(power(TCW1,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000)) =e= 0;
198  EQU28..H12-(H11-Q102) =e= 0;
199  EQU29..TE102-(((T11-TCW2)-(T12-TCW1))/log((T11-TCW2)/(T12-TCW1))) =e= 0;
200  EQU30..Q102-areaE102*uE102*TE102/1000000 =e= 0;
201  EQU31..f12-(f12h2+f12n2+f12nh3+f12h2o+f12ph+f12an+f12dpa) =e= 0;
202  EQU32..f13h2-f12h2 =e= 0;
203  EQU33..f13n2-f12n2 =e= 0;
204  EQU34..f13nh3-0.999*f12nh3 =e= 0;
205  EQU35..f03-f03nh3 =e= 0;
206  EQU36..H03-(f03nh3*(hfnh3+sum(coeff2,enth_liq("nh3",coeff2)*(power(T03,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000) =e=
                                                                                                                    0;
207  EQU37..f04-f04ph =e= 0;
208  EQU38..f07h2-f16h2 =e= 0;
209  EQU39..f07n2-f16n2 =e= 0;
210  EQU40..f07nh3-(f03nh3+f16nh3) =e= 0;
211  EQU41..f07h2o-f16h2o =e= 0;
212  EQU42..f07ph-(f04ph+f31ph) =e= 0;
213  EQU43..f07an-f31an =e= 0;
214  EQU44..f07dpa-f31dpa =e= 0;
215  EQU45..H04-(f04ph*(hfph+sum(coeff2,enth_liq("ph",coeff2)*(power(T04,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000) =e= 0;
216  EQU46..f07-(f07h2+f07n2+f07nh3+f07h2o+f07ph+f07an+f07dpa) =e= 0;
217  EQU47..H07-((f07h2*(hfh2+sum(coeff1,enth_gas("h2",coeff1)*(power(T07,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
218  (f07n2*(hfn2+sum(coeff1,enth_gas("n2",coeff1)*(power(T07,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
219  (f07nh3*(hfnh3+sum(coeff1,enth_gas("nh3",coeff1)*(power(T07,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
220  (f07h2o*(hfh2o+sum(coeff1,enth_gas("h2o",coeff1)*(power(T07,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
221  (f07ph*(hfph+sum(coeff2,enth_liq("ph",coeff2)*(power(T07,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000) +
222  (f07an*(hfan+sum(coeff2,enth_liq("an",coeff2)*(power(T07,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000) +
223  (f07dpa*(hfdpa+sum(coeff2,enth_liq("dpa",coeff2)*(power(T07,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000)) =e= 0;
224  EQU48..f08h2-f07h2 =e= 0;
225  EQU49..f08n2-f07n2 =e= 0;
226  EQU50..f08nh3-f07nh3 =e= 0;
227  EQU51..f08h2o-f07h2o =e= 0;
228  EQU52..f08ph-f07ph =e= 0;
229  EQU53..f08an-f07an =e= 0;
230  EQU54..f08dpa-f07dpa =e= 0;
231  EQU55..f08-(f08h2+f08n2+f08nh3+f08h2o+f08ph+f08an+f08dpa) =e= 0;
232  EQU56..H08-((f08h2*(hfh2+sum(coeff1,enth_gas("h2",coeff1)*(power(T08,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
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233  (f08n2*(hfn2+sum(coeff1,enth_gas("n2",coeff1)*(power(T08,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
234  (f08nh3*(hfnh3+sum(coeff1,enth_gas("nh3",coeff1)*(power(T08,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
235  (f08h2o*(hfh2o+sum(coeff1,enth_gas("h2o",coeff1)*(power(T08,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
236  (f08ph*(hfph+sum(coeff1,enth_gas("ph",coeff1)*(power(T08,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
237  (f08an*(hfan+sum(coeff1,enth_gas("an",coeff1)*(power(T08,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
238  (f08dpa*(hfdpa+sum(coeff1,enth_gas("dpa",coeff1)*(power(T08,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000)) =e= 0;
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 239  EQU57..f09h2-f08h2 =e= 0;
 240  EQU58..f09n2-f08n2 =e= 0;
 241  EQU59..f09nh3-f08nh3 =e= 0;
 242  EQU60..f09h2o-f08h2o =e= 0;
 243  EQU61..f09ph-f08ph =e= 0;
 244  EQU62..f09an-f08an =e= 0;
 245  EQU63..f09dpa-f08dpa =e= 0;
 246  EQU64..Q101-(H09-H08) =e= 0;
 247  EQU65..f09-(f09h2+f09n2+f09nh3+f09h2o+f09ph+f09an+f09dpa) =e= 0;
 248  EQU66..H09-((f09h2*(hfh2+sum(coeff1,enth_gas("h2",coeff1)*(power(T09,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
 249  (f09n2*(hfn2+sum(coeff1,enth_gas("n2",coeff1)*(power(T09,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
 250  (f09nh3*(hfnh3+sum(coeff1,enth_gas("nh3",coeff1)*(power(T09,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
 251  (f09h2o*(hfh2+sum(coeff1,enth_gas("h2o",coeff1)*(power(T09,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
 252  (f09ph*(hfph+sum(coeff1,enth_gas("ph",coeff1)*(power(T09,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
 253  (f09an*(hfan+sum(coeff1,enth_gas("an",coeff1)*(power(T09,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
 254  (f09dpa*(hfdpa+sum(coeff1,enth_gas("dpa",coeff1)*(power(T09,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000)) =e= 0;
 255  EQU67..f10nh3-((1-conv2)*f09nh3-0.995*conv1*f09ph) =e= 0;
 256  EQU68..f10h2o-(f09h2o+conv1*f09ph) =e= 0;
 257  EQU69..f10h2-(f09h2+1.5*conv2*f09nh3) =e= 0;
 258  EQU70..f10n2-(f09n2+0.5*conv2*f09nh3) =e= 0;
 259  EQU71..feed_h2-(1000*f09h2*dens_h2/(f09*h2)) =e= 0;
 260  EQU72..feed_n2-(1000*f09n2*dens_n2/(f09*n2)) =e= 0;
 261  EQU73..feed_nh3-(1000*f09nh3*dens_nh3/(f09*nh3)) =e= 0;
 262  EQU74..feed_h2o-(1000*f09h2o*dens_h2o/(f09*h2o)) =e= 0;
 263  EQU75..feed_ph-(1000*f09ph*dens_ph/(f09*ph)) =e= 0;
 264  EQU76..feed_an-(1000*f09an*dens_an/(f09*an)) =e= 0;
 265  EQU77..feed_dpa-(1000*f09dpa*dens_dpa/(f09*dpa)) =e= 0;
 266  EQU78..eff_h2-(1000*f10h2*dens_h2/(f10*h2)) =e= 0;
 267  EQU79..eff_n2-(1000*f10n2*dens_n2/(f10*n2)) =e= 0;
 268  EQU80..eff_nh3-(1000*f10nh3*dens_nh3/(f10*nh3)) =e= 0;
 269  EQU81..f13h2o-0.100*f12h2o =e= 0;
 270  EQU82..f13-(f13h2+f13n2+f13nh3+f13h2o) =e= 0;
 271  EQU83..H13-((f13h2*(hfh2+sum(coeff1,enth_gas("h2",coeff1)*(power(T13,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
 272  (f13n2*(hfn2+sum(coeff1,enth_gas("n2",coeff1)*(power(T13,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
 273  (f13nh3*(hfnh3+sum(coeff1,enth_gas("nh3",coeff1)*(power(T13,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
 274  (f13h2o*(hfh2o+sum(coeff1,enth_gas("h2o",coeff1)*(power(T13,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000)) =e= 0;
 275  EQU84..f14h2-0.989*f13h2 =e= 0;
 276  EQU85..f14n2-0.989*f13n2 =e= 0;
 277  EQU86..f14nh3-0.989*f13nh3 =e= 0;
 278  EQU87..f14h2o-0.989*f13h2o =e= 0;
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 279  EQU88..H14-0.989*H13 =e=0;
 280  EQU89..T14-T13 =e= 0;
 281  EQU90..f14-(f14h2+f14n2+f14nh3+f14h2o) =e= 0;
 282  EQU91..f16h2-f14h2 =e= 0;
 283  EQU92..f16n2-f14n2 =e= 0;
 284  EQU93..f16nh3-f14nh3 =e= 0;
 285  EQU94..f16h2o-f14h2o =e= 0;
 286  EQU95..f16-(f16h2+f16n2+f16nh3+f16h2o) =e= 0;
 287  EQU96..H16-((f16h2*(hfh2+sum(coeff1,enth_gas("h2",coeff1)*(power(T16,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
 288  (f16n2*(hfn2+sum(coeff1,enth_gas("n2",coeff1)*(power(T16,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
 289  (f16nh3*(hfnh3+sum(coeff1,enth_gas("nh3",coeff1)*(power(T16,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
 290  (f16h2o*(hfh2o+sum(coeff1,enth_gas("h2o",coeff1)*(power(T16,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000)) =e= 0;
 291  EQU97..f17h2-0.011*f13h2 =e= 0;
 292  EQU98..f17n2-0.011*f13n2 =e= 0;
 293  EQU99..f17nh3-0.011*f13nh3 =e= 0;
 294  EQU100..f17h2o-0.011*f13h2o =e= 0;
 295  EQU101..H17-0.011*H13 =e= 0;
 296  EQU102..T17-T13 =e= 0;
 297  EQU103..f17-(f17h2+f17n2+f17nh3+f17h2o) =e= 0;
 298  EQU104..f18nh3-0.0001*f12nh3 =e= 0;
 299  EQU105..f18h2o-0.900*f12h2o =e= 0;
 300  EQU106..f18ph-f12ph =e= 0;
 301  EQU107..f18an-f12an =e= 0;
 302  EQU108..f18dpa-f12dpa =e= 0;
 303  EQU109..f18-(f18nh3+f18h2o+f18ph+f18an+f18dpa) =e= 0;
 304  EQU110..H18-((f18nh3*(hfnh3+sum(coeff2,enth_liq("nh3",coeff2)*(power(T18,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000) +
 305  (f18h2o*(hfh2o+sum(coeff2,enth_liq("h2o",coeff2)*(power(T18,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000) +
 306  (f18ph*(hfph+sum(coeff2,enth_liq("ph",coeff2)*(power(T18,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000) +
 307  (f18an*(hfan+sum(coeff2,enth_liq("an",coeff2)*(power(T18,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000) +
 308  (f18dpa*(hfdpa+sum(coeff2,enth_liq("dpa",coeff2)*(power(T18,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000)) =e= 0;
 309  EQU111..f19nh3-(f18nh3+f23nh3) =e= 0;
 310  EQU112..f19h2o-0.9999*(f18h2o+f23h2o) =e= 0;
 311  EQU113..f19ph-0.060*(f18ph+f23ph) =e= 0;
 312  EQU114..f19an-0.050*(f18an+f23an) =e= 0;
 313  EQU115..f19-(f19nh3+f19h2o+f19ph+f19an) =e= 0;
 314  EQU116..H19-((f19nh3*(hfnh3+sum(coeff1,enth_gas("nh3",coeff1)*(power(T19,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
 315  (f19h2o*(hfh2o+sum(coeff1,enth_gas("h2o",coeff1)*(power(T19,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
 316  (f19ph*(hfph+sum(coeff1,enth_gas("ph",coeff1)*(power(T19,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000) +
 317  (f19an*(hfan+sum(coeff1,enth_gas("an",coeff1)*(power(T19,ord(coeff1))-power(536.67,ord(coeff1)))))/1000000)) =e= 0;
 318  EQU117..f20nh3-f19nh3 =e= 0;
 319  EQU118..f20h2o-f19h2o =e= 0;
 320  EQU119..f20ph-f19ph =e= 0;
 321  EQU120..f20an-f19an =e= 0;
 322  EQU121..fCW4-fCW3 =e= 0;
 323  EQU122..Q103-((fCW4*(hfh2o+sum(coeff2,enth_liq("h2o",coeff2)*(power(TCW4,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000) -
 324  (fCW3*(hfh2o+sum(coeff2,enth_liq("h2o",coeff2)*(power(TCW3,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000)) =e= 0;
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 325  EQU123..H20-(H19-Q103) =e= 0;
 326  EQU124..TE103-(((T19-TCW4)-(T20-TCW3))/log((T19-TCW4)/(T20-TCW3))) =e= 0;
 327  EQU125..Q103-areaE103*uE103*TE103/1000000 =e= 0;
 328  EQU126..f20-(f20nh3+f20h2o+f20ph+f20an) =e= 0;
 329  EQU127..f21nh3-0.070*f20nh3 =e= 0;
 330  EQU128..f21h2o-0.030*f20h2o =e= 0;
 331  EQU129..f21ph-0.305*f20ph =e= 0;
 332  EQU130..f21an-0.860*f20an =e= 0;
 333  EQU131..f21-(f21nh3+f21h2o+f21ph+f21an) =e= 0;
 334  EQU132..H21-((f21nh3*(hfnh3+sum(coeff2,enth_liq("nh3",coeff2)*(power(T21,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 335  (f21h2o*(hfh2o+sum(coeff2,enth_liq("h2o",coeff2)*(power(T21,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 336  (f21ph*(hfph+sum(coeff2,enth_liq("ph",coeff2)*(power(T21,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 337  (f21an*(hfan+sum(coeff2,enth_liq("an",coeff2)*(power(T21,ord(coeff2))-power(536.67,ord(coeff2))))/1000000)) =e= 0;
 338  EQU133..T21-T20 =e= 0;
 339  EQU134..f23nh3-f21nh3 =e= 0;
 340  EQU135..f23h2o-f21h2o =e= 0;
 341  EQU136..f23ph-f21ph =e= 0;
 342  EQU137..f23an-f21an =e= 0;
 343  EQU138..f23-(f23nh3+f23h2o+f23ph+f23an) =e= 0;
 344  EQU139..H23-((f23nh3*(hfnh3+sum(coeff2,enth_liq("nh3",coeff2)*(power(T23,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 345  (f23h2o*(hfh2o+sum(coeff2,enth_liq("h2o",coeff2)*(power(T23,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 346  (f23ph*(hfph+sum(coeff2,enth_liq("ph",coeff2)*(power(T23,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 347  (f23an*(hfan+sum(coeff2,enth_liq("an",coeff2)*(power(T23,ord(coeff2))-power(536.67,ord(coeff2))))/1000000)) =e= 0;
 348  EQU140..f24nh3-0.930*f20nh3 =e= 0;
 349  EQU141..f24h2o-0.970*f20h2o =e= 0;
 350  EQU142..f24ph-0.695*f20ph =e= 0;
 351  EQU143..f24an-0.140*f20an =e= 0;
 352  EQU144..T24-T20 =e= 0;
 353  EQU145..f24-(f24nh3+f24h2o+f24ph+f24an) =e= 0;
 354  EQU146..H24-((f24nh3*(hfnh3+sum(coeff2,enth_liq("nh3",coeff2)*(power(T24,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 355  (f24h2o*(hfh2o+sum(coeff2,enth_liq("h2o",coeff2)*(power(T24,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 356  (f24ph*(hfph+sum(coeff2,enth_liq("ph",coeff2)*(power(T24,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 357  (f24an*(hfan+sum(coeff2,enth_liq("an",coeff2)*(power(T24,ord(coeff2))-power(536.67,ord(coeff2))))/1000000)) =e= 0;
 358  EQU147..f25h2o-0.0001*(f18h2o+f23h2o) =e= 0;
 359  EQU148..f25ph-0.940*(f18ph+f23ph) =e= 0;
 360  EQU149..f25an-0.949*(f18an+f23an) =e= 0;
 361  EQU150..f25dpa-f18dpa =e= 0;
 362  EQU151..f25-(f25h2o+f25ph+f25an+f25dpa) =e= 0;
 363  EQU152..H25-((f25h2o*(hfh2o+sum(coeff2,enth_liq("h2o",coeff2)*(power(T25,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 364  (f25ph*(hfph+sum(coeff2,enth_liq("ph",coeff2)*(power(T25,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 365  (f25an*(hfan+sum(coeff2,enth_liq("an",coeff2)*(power(T25,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 366  (f25dpa*(hfdpa+sum(coeff2,enth_liq("dpa",coeff2)*(power(T25,ord(coeff2))-power(536.67,ord(coeff2))))/1000000)) =e= 0;
 367  EQU153..f26h2o-f25h2o =e= 0;
 368  EQU154..f26ph-0.195*f25ph =e= 0;
 369  EQU155..f26an-0.923*f25an =e= 0;
 370  EQU156..f26-(f26h2o+f26ph+f26an) =e= 0;
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 371  EQU157..H26-((f26h2o*(hfh2o+sum(coeff2,enth_liq("h2o",coeff2)*(power(T26,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 372  (f26ph*(hfph+sum(coeff2,enth_liq("ph",coeff2)*(power(T26,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 373  (f26an*(hfan+sum(coeff2,enth_liq("an",coeff2)*(power(T26,ord(coeff2))-power(536.67,ord(coeff2))))/1000000)) =e= 0;
 374  EQU158..f27h2o-f26h2o =e= 0;
 375  EQU159..f27ph-f26ph =e= 0;
 376  EQU160..f27an-f26an =e= 0;
 377  EQU161..f27-(f27h2o+f27ph+f27an) =e= 0;
 378  EQU162..H27-((f27h2o*(hfh2o+sum(coeff2,enth_liq("h2o",coeff2)*(power(T27,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 379  (f27ph*(hfph+sum(coeff2,enth_liq("ph",coeff2)*(power(T27,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 380  (f27an*(hfan+sum(coeff2,enth_liq("an",coeff2)*(power(T27,ord(coeff2))-power(536.67,ord(coeff2))))/1000000)) =e= 0;
 381  EQU163..f28h2o-f27h2o =e= 0;
 382  EQU164..f28ph-f27ph =e= 0;
 383  EQU165..f28an-f27an =e= 0;
 384  EQU166..fCW6-fCW5 =e= 0;
 385  EQU167..Q104-((fCW6*(hfh2o+sum(coeff2,enth_liq("h2o",coeff2)*(power(TCW6,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) -
 386  (fCW5*(hfh2o+sum(coeff2,enth_liq("h2o",coeff2)*(power(TCW5,ord(coeff2))-power(536.67,ord(coeff2))))/1000000)) =e= 0;
 387  EQU168..H28-(H27-Q104) =e= 0;
 388  EQU169..TE104-(((T27-TCW6)-(T28-TCW5))/log((T27-TCW6)/(T28-TCW5))) =e= 0;
 389  EQU170..Q104-areaE104*uE104*TE104/1000000 =e= 0;
 390  EQU171..f28-(f28h2o+f28ph+f28an) =e= 0;
 391  EQU172..f29ph-0.800*f25ph =e= 0;
 392  EQU173..f29an-0.077*f25an =e= 0;
 393  EQU174..f29dpa-0.046*f25dpa =e= 0;
 394  EQU175..f29-(f29ph+f29an+f29dpa) =e= 0;
 395  EQU176..H29-((f29ph*(hfph+sum(coeff2,enth_liq("ph",coeff2)*(power(T29,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 396  (f29an*(hfan+sum(coeff2,enth_liq("an",coeff2)*(power(T29,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 397  (f29dpa*(hfdpa+sum(coeff2,enth_liq("dpa",coeff2)*(power(T29,ord(coeff2))-power(536.67,ord(coeff2))))/1000000)) =e= 0;
 398  EQU177..f31ph-f29ph =e= 0;
 399  EQU178..f31an-f29an =e= 0;
 400  EQU179..f31dpa-f29dpa =e= 0;
 401  EQU180..f31-(f31ph+f31an+f31dpa) =e= 0;
 402  EQU181..H31-((f31ph*(hfph+sum(coeff2,enth_liq("ph",coeff2)*(power(T31,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 403  (f31an*(hfan+sum(coeff2,enth_liq("an",coeff2)*(power(T31,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 404  (f31dpa*(hfdpa+sum(coeff2,enth_liq("dpa",coeff2)*(power(T31,ord(coeff2))-power(536.67,ord(coeff2))))/1000000)) =e= 0;
 405  EQU182..f32ph-0.005*f25ph =e= 0;
 406  EQU183..f32an-0.000246*f25an =e= 0;
 407  EQU184..f32dpa-0.954*f25dpa =e= 0;
 408  EQU185..f32-(f32ph+f32an+f32dpa) =e= 0;
 409  EQU186..H32-((f32ph*(hfph+sum(coeff2,enth_liq("ph",coeff2)*(power(T32,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
 410  (f32an*(hfan+sum(coeff2,enth_liq("an",coeff2)*(power(T32,ord(coeff2))-power(536.67,ord(coeff2))))/1000000) +
```

```
 411  (f32dpa*(hfdpa+sum(coeff2,enth_liq("dpa",coeff2)*(power(T32,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000)) =e= 0;
 412  EQU187..f33ph-f32ph =e= 0;
 413  EQU188..f33an-f32an =e= 0;
 414  EQU189..f33dpa-f32dpa =e= 0;
 415  EQU190..fCW8-fCW7 =e= 0;
 416  EQU191..Q105-((fCW8*(hfh2o+sum(coeff2,enth_liq("h2o",coeff2)*(power(TCW8,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000) -
Economic Optimization Program                                                    02/12/01 09:49:34  PAGE     10
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 417  (fCW7*(hfh2o+sum(coeff2,enth_liq("h2o",coeff2)*(power(TCW7,ord(coeff2))-power(536.67,ord(coeff2)))))/1000000)) =e= 0;
 418  EQU192..H33-(H32-Q105) =e= 0;
 419  EQU193..TE105-(((T32-TCW8)-(T33-TCW7))/log((T32-TCW8)/(T33-TCW7))) =e= 0;
 420  EQU194..Q105-areaE105*uE105*TE105/1000000 =e= 0;
 421  EQU195..f33-(f33ph+f33an+f33dpa) =e= 0;
 422  EQU196..profit-(price_an*f28*an+price_dpa*f33*dpa-price_nh3*f03*nh3-price_ph*f04*ph) =e= 0;
 423  EQU197..eff_h2o-(1000*f10h2o*dens_h2o/(f10*h2o)) =e= 0;
 424  EQU198..eff_ph-(1000*f10ph*dens_ph/(f10*ph)) =e= 0;
 425  EQU199..eff_an-(1000*f10an*dens_an/(f10*an)) =e= 0;
 426  EQU200..eff_dpa-(1000*f10dpa*dens_dpa/(f10*dpa)) =e= 0;
 427
 428  INEQU1..f07nh3/f07ph =g= 15;
 429  INEQU2..T10-T08 =g= 75;
 430  INEQU3..T12-TCW1 =g= 60;
 431  INEQU4..T20-TCW3 =g= 30;
 432  INEQU5..f26an-(0.989*(f26h2o*h2o+f26ph*ph+f26an*an)/an) =g= 0;
 433  INEQU6..T28-TCW5 =g= 10;
 434  INEQU7..f29ph-(0.300*(f29ph*ph+f29an*an+f29dpa*dpa)/ph) =g= 0;
 435  INEQU8..f29an-(0.650*(f29ph*ph+f29an*an+f29dpa*dpa)/an) =g= 0;
 436  INEQU9..T33-TCW7 =g= 50;
 437  INEQU10..f32dpa-(0.945*(f32ph*ph+f32an*an+f32dpa*dpa)/dpa) =g= 0;
 438
 439  f03.L=203; f04.L=165.7; f07.L=4250;
 440  f08.L=4250; f09.L=4250; f10.L=4250;
 441  f11.L=4250; f12.L=4250; f13.L=3900;
 442  f14.L=3860; f16.L=3860; f17.L=43;
 443  f18.L=345; f19.L=180; f20.L=180;
 444  f21.L=13; f23.L=13; f24.L=170;
 445  f25.L=180; f26.L=162.4; f27.L=162.4;
 446  f28.L=162.4; f29.L=15; f31.L=15;
 447  f32.L=0.9; f33.L=0.9; fCW1.L=22900;
 448  fCW2.L=22900; fCW3.L=9700; fCW4.L=9700;
 449  fCW5.L=3400; fCW6.L=3400; fCW7.L=80;
 450  fCW8.L=80; T03.L=550; T04.L=570;
 451  T07.L=615; T08.L=1125; T09.L=1185;
 452  T10.L=1200; T11.L=680; T12.L=600;
 453  T13.L=600; T14.L=600; T16.L=630;
 454  T17.L=600; T18.L=825; T19.L=675;
 455  T20.L=570; T21.L=570; T23.L=570;
 456  T24.L=570; T25.L=850; T26.L=725;
 457  T27.L=725; T28.L=550; T29.L=830;
 458  T31.L=835; T32.L=1010; T33.L=590;
 459  TCW1.L=540; TCW2.L=560; TCW3.L=540;
 460  TCW4.L=560; TCW5.L=540; TCW6.L=560;
 461  TCW7.L=540; TCW8.L=560;
 462  f03.LO=200; f04.LO=160; f07.LO=4240;
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 463  f08.LO=4240; f09.LO=4240; f10.LO=4240;
 464  f11.LO=4240; f12.LO=4240; f13.LO=3890;
 465  f14.LO=3850; f16.LO=3850; f17.LO=40;
 466  f18.LO=330; f19.LO=170; f20.LO=170;
 467  f21.LO=12; f23.LO=12; f24.LO=160;
 468  f25.LO=170; f26.LO=160; f27.LO=160;
 469  f28.LO=160; f29.LO=10; f31.LO=10;
 470  f32.LO=0.8; f33.LO=0.8; fCW1.LO=22000;
 471  fCW2.LO=22000; fCW3.LO=9600; fCW4.LO=9600;
 472  fCW5.LO=3350; fCW6.LO=3350; fCW7.LO=75;
 473  fCW8.LO=75; T03.LO=540; T04.LO=560;
 474  T07.LO=605; T08.LO=1120; T09.LO=1175;
 475  T10.LO=1195; T11.LO=670; T12.LO=590;
 476  T13.LO=590; T14.LO=590; T16.LO=620;
 477  T17.LO=590; T18.LO=815; T19.LO=665;
 478  T20.LO=560; T21.LO=560; T23.LO=560;
 479  T24.LO=560; T25.LO=840; T26.LO=715;
 480  T27.LO=715; T28.LO=545; T29.LO=820;
 481  T31.LO=825; T32.LO=1000; T33.LO=580;
 482  TCW1.LO=535; TCW2.LO=555; TCW3.LO=535;
 483  TCW4.LO=555; TCW5.LO=535; TCW6.LO=555;
 484  TCW7.LO=535; TCW8.LO=555;
 485  f03.UP=205; f04.UP=170; f07.UP=4300;
 486  f08.UP=4300; f09.UP=4300; f10.UP=4300;
 487  f11.UP=4300; f12.UP=4300; f13.UP=3950;
 488  f14.UP=3900; f16.UP=3900; f17.UP=45;
 489  f18.UP=360; f19.UP=190; f20.UP=190;
 490  f21.UP=14; f23.UP=14; f24.UP=190;
 491  f25.UP=190; f26.UP=165; f27.UP=165;
 492  f28.UP=165; f29.UP=20; f31.UP=20;
 493  f32.UP=1; f33.UP=1; fCW1.UP=24000;
 494  fCW2.UP=24000; fCW3.UP=9800; fCW4.UP=9800;
```

```
 495  fCW5.UP=3450; fCW6.UP=3450; fCW7.UP=85;
 496  fCW8.UP=85; T03.UP=560; T04.UP=580;
 497  T07.UP=625; T08.UP=1130; T09.UP=1195;
 498  T10.UP=1205; T11.UP=690; T12.UP=610;
 499  T13.UP=610; T14.UP=610; T16.UP=640;
 500  T17.UP=610; T18.UP=835; T19.UP=685;
 501  T20.UP=580; T21.UP=580; T23.UP=580;
 502  T24.UP=580; T25.UP=860; T26.UP=735;
 503  T27.UP=735; T28.UP=555; T29.UP=840;
 504  T31.UP=845; T32.UP=1020; T33.UP=600;
 505  TCW1.UP=545; TCW2.UP=565; TCW3.UP=545;
 506  TCW4.UP=565; TCW5.UP=545; TCW6.UP=565;
 507  TCW7.UP=545; TCW8.UP=565;
 508
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 509
 510
 511  f03nh3.L=203; f04ph.L=165;
 512  f07h2.L=480;
 513  f07n2.L=160; f07nh3.L=3450;
 514  f07ph.L=170;
 515  f08h2.L=480; f08n2.L=160;
 516  f08nh3.L=3450;
 517  f09h2.L=480;
 518  f09n2.L=160; f09nh3.L=3450;
 519  f10h2.L=485;
 520  f10nh3.L=3280;
 521
 522  f11n2.L=162;
 523  f11nh3.L=3280;
 524
 525  f12n2.L=162; f12nh3.L=3280;
 526  f13h2.L=485; f13n2.L=160;
 527  f13nh3.L=3279; f14h2.L=480;
 528  f14n2.L=160; f14nh3.L=3240; f16h2.L=480;
 529  f16n2.L=160; f16nh3.L=3240;
 530  f17n2.L=1.8;
 531  f17nh3.L=36.1;
 532
 533
 534
 535
 536
 537
 538  f23ph.L=0.1;
 539
 540
 541  f26ph.L=1.6;
 542  f27ph.L=1.6;
 543  f28ph.L=1.6;
 544  f29an.L=10;
 545  f31ph.L=5;
 546
 547
 548
 549
 550  H03.L=-4; H04.L=-6.5;
 551  H07.L=-73; H08.L=-50; H09.L=-46;
 552  H10.L=-46;
 553  H13.L=-65; H14.L=-64; H16.L=-63;
 554  H17.L=-1; H18.L=-7;
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 555  H21.L=-0.2; H23.L=-0.2;
 556  H24.L=-17; H25.L=9; H26.L=7.5;
 557  H28.L=6.2; H29.L=0.5;
 558  H31.L=0.5;
 559
 560
 561  TE102.L=90;
 562  TE103.L=65; TE104.L=55; TE105.L=180;
 563  eff_an.LO=0.0001; eff_dpa.LO=0.0001; eff_h2.LO=0.0001;
 564  eff_h2o.LO=0.0001; eff_n2.LO=0.0001; eff_nh3.LO=0.0001;
 565  eff_ph.LO=0.0001; f03nh3.LO=0.0001; f04ph.LO=0.0001;
 566  f07an.LO=0.0001; f07dpa.LO=0.0001; f07h2.LO=0.0001;
 567  f07h2o.LO=0.0001; f07n2.LO=0.0001; f07nh3.LO=0.0001;
 568  f07ph.LO=0.0001; f08an.LO=0.0001; f08dpa.LO=0.0001;
 569  f08h2.LO=0.0001; f08h2o.LO=0.0001; f08n2.LO=0.0001;
 570  f08nh3.LO=0.0001; f08ph.LO=0.0001; f09an.LO=0.0001;
 571  f09dpa.LO=0.0001; f09h2.LO=0.0001; f09h2o.LO=0.0001;
 572  f09n2.LO=0.0001; f09nh3.LO=0.0001; f09ph.LO=0.0001;
 573  f10an.LO=0.0001; f10dpa.LO=0.0001; f10h2.LO=0.0001;
 574  f10h2o.LO=0.0001; f10n2.LO=0.0001; f10nh3.LO=0.0001;
 575  f10ph.LO=0.0001; f11an.LO=0.0001; f11dpa.LO=0.0001;
 576  f11h2.LO=0.0001; f11h2o.LO=0.0001; f11n2.LO=0.0001;
 577  f11nh3.LO=0.0001; f11ph.LO=0.0001; f12an.LO=0.0001;
 578  f12dpa.LO=0.0001; f12h2.LO=0.0001; f12h2o.LO=0.0001;
```

```
 579  f12n2.LO=0.0001; f12nh3.LO=0.0001; f12ph.LO=0.0001;
 580  f13h2.LO=0.0001; f13h2o.LO=0.0001; f13n2.LO=0.0001;
 581  f13nh3.LO=0.0001; f14h2.LO=0.0001; f14h2o.LO=0.0001;
 582  f14n2.LO=0.0001; f14nh3.LO=0.0001; f16h2.LO=0.0001;
 583  f16h2o.LO=0.0001; f16n2.LO=0.0001; f16nh3.LO=0.0001;
 584  f17h2.LO=0.0001; f17h2o.LO=0.0001; f17n2.LO=0.0001;
 585  f17nh3.LO=0.0001; f18an.LO=0.0001; f18dpa.LO=0.0001;
 586  f18h2o.LO=0.0001; f18nh3.LO=0.0001; f18ph.LO=0.0001;
 587  f19an.LO=0.0001; f19h2o.LO=0.0001; f19nh3.LO=0.0001;
 588  f19ph.LO=0.0001; f20an.LO=0.0001; f20h2o.LO=0.0001;
 589  f20nh3.LO=0.0001; f20ph.LO=0.0001; f21an.LO=0.0001;
 590  f21h2o.LO=0.0001; f21nh3.LO=0.0001; f21ph.LO=0.0001;
 591  f23an.LO=0.0001; f23h2o.LO=0.0001; f23nh3.LO=0.0001;
 592  f23ph.LO=0.0001; f24an.LO=0.0001; f24h2o.LO=0.0001;
 593  f24nh3.LO=0.0001; f24ph.LO=0.0001; f25an.LO=0.0001;
 594  f25dpa.LO=0.0001; f25h2o.LO=0.0001; f25ph.LO=0.0001;
 595  f26an.LO=0.0001; f26h2o.LO=0.0001; f26ph.LO=0.0001;
 596  f27an.LO=0.0001; f27h2o.LO=0.0001; f27ph.LO=0.0001;
 597  f28an.LO=0.0001; f28h2o.LO=0.0001; f28ph.LO=0.0001;
 598  f29an.LO=0.0001; f29dpa.LO=0.0001; f29ph.LO=0.0001;
 599  f31an.LO=0.0001; f31dpa.LO=0.0001; f31ph.LO=0.0001;
 600  f32an.LO=0.0001; f32dpa.LO=0.0001; f32ph.LO=0.0001;
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 601  f33an.LO=0.0001; f33dpa.LO=0.0001; f33ph.LO=0.0001;
 602  feed_an.LO=0.0001; feed_dpa.LO=0.0001; feed_h2.LO=0.0001;
 603  feed_h2o.LO=0.0001; feed_n2.LO=0.0001; feed_nh3.LO=0.0001;
 604  feed_ph.LO=0.0001; H03.LO=-9999; H04.LO=-9999;
 605  H07.LO=-9999; H08.LO=-9999; H09.LO=-9999;
 606  H10.LO=-9999; H11.LO=-9999; H12.LO=-9999;
 607  H13.LO=-9999; H14.LO=-9999; H16.LO=-9999;
 608  H17.LO=-9999; H18.LO=-9999; H19.LO=-9999;
 609  H20.LO=-9999; H21.LO=-9999; H23.LO=-9999;
 610  H24.LO=-9999; H25.LO=-9999; H26.LO=-9999;
 611  H27.LO=-9999; H28.LO=-9999; H29.LO=-9999;
 612  H31.LO=-9999; H32.LO=-9999; H33.LO=-9999;
 613  profit.LO=0.0001; Q100.LO=-9999; Q101.LO=-9999;
 614  Q102.LO=-9999; Q103.LO=-9999; Q104.LO=-9999;
 615  Q105.LO=-9999; TE100.LO=0; TE102.LO=0;
 616  TE103.LO=0; TE104.LO=0; TE105.LO=0;
 617
 618
 619  MODEL Aniline /ALL/;
 620  OPTION LIMCOL=0;
 621  OPTION LIMROW=0;
 622  OPTION ITERLIM= 100;
 623  OPTION DOMLIM= 0;
 624  OPTION RESLIM= 1000;
 625
 626  OPTION NLP=CONOPT;
 627  SOLVE Aniline Using NLP Maximizing ObjVar;
 628


COMPILATION TIME     =        0.060 SECONDS    0.8 Mb      WIN-18-097
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Model Statistics    SOLVE ANILINE USING NLP FROM LINE 627                GAMS 2.50A    Windows NT/95/98



MODEL STATISTICS

BLOCKS OF EQUATIONS     211     SINGLE EQUATIONS     211
BLOCKS OF VARIABLES     231     SINGLE VARIABLES     231
NON ZERO ELEMENTS       653     NON LINEAR N-Z       163
DERIVATIVE POOL          12     CONSTANT POOL         85
CODE LENGTH            7545


GENERATION TIME      =        0.050 SECONDS    1.5 Mb      WIN-18-097


EXECUTION TIME       =        0.050 SECONDS    1.5 Mb      WIN-18-097
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          S O L V E     S U M M A R Y

     MODEL   ANILINE          OBJECTIVE  OBJVAR
     TYPE    NLP            DIRECTION  MAXIMIZE
     SOLVER  CONOPT           FROM LINE  627

**** SOLVER STATUS     1 NORMAL COMPLETION
**** MODEL STATUS      2 LOCALLY OPTIMAL
**** OBJECTIVE VALUE           1402.2768

 RESOURCE USAGE, LIMIT         0.109     1000.000
 ITERATION COUNT, LIMIT        18        100
```

```
EVALUATION ERRORS            0          0

    C O N O P T   Wintel  version 2.042F-003-035
    Copyright (C) ARKI Consulting and Development A/S
                  Bagsvaerdvej 246 A
                  DK-2880 Bagsvaerd, Denmark

Using default control program.


** Optimal solution. Reduced gradient less than tolerance.


CONOPT time Total                    0.059 seconds
  of which: Function evaluations      0.000 =  0.0%
            Derivative evaluations    0.000 =  0.0%

Work length =     0.36 Mbytes
   Estimate =     0.36 Mbytes
   Max used =     0.16 Mbytes

                    LOWER        LEVEL        UPPER       MARGINAL

---- EQU EQU1            .            .            .         37.3272
---- EQU EQU2            .            .            .         45.2379
---- EQU EQU3            .            .            .        304.2000
---- EQU EQU4            .            .            .            EPS
---- EQU EQU5         15.0000      15.0000      15.0000        EPS
---- EQU EQU6            .            .            .            EPS
---- EQU EQU7            .            .            .         10.5257
---- EQU EQU8            .            .            .         10.5257
---- EQU EQU9            .            .            .         10.5160
---- EQU EQU10           .            .            .          0.0175
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                    LOWER        LEVEL        UPPER       MARGINAL

---- EQU EQU11           .            .            .         37.3272
---- EQU EQU12           .            .            .         45.2379
---- EQU EQU13           .            .            .        304.2000
---- EQU EQU14           .            .            .            EPS
---- EQU EQU15           .            .            .            EPS
---- EQU EQU16           .            .            .            EPS
---- EQU EQU17           .            .            .            EPS
---- EQU EQU18           .            .            .            EPS
---- EQU EQU19           .            .            .         10.5257

---- EQU EQU20           .            .            .         10.5257
---- EQU EQU21           .            .            .         10.5160
---- EQU EQU22           .            .            .          0.0175
---- EQU EQU23           .            .            .         37.3272
---- EQU EQU24           .            .            .         45.2379
---- EQU EQU25           .            .            .        304.2000
---- EQU EQU26           .            .            .            EPS
---- EQU EQU27           .            .            .            EPS
---- EQU EQU28           .            .            .            EPS
---- EQU EQU29           .            .            .            EPS
---- EQU EQU30           .            .            .            EPS
---- EQU EQU31           .            .            .            EPS
---- EQU EQU32           .            .            .         10.5257
---- EQU EQU33           .            .            .         10.5257
---- EQU EQU34           .            .            .         10.5265
---- EQU EQU35           .            .            .        -10.5265
---- EQU EQU36           .            .            .            EPS
---- EQU EQU37           .            .            .        -35.7200
---- EQU EQU38           .            .            .         10.5257
---- EQU EQU39           .            .            .         10.5257
---- EQU EQU40           .            .            .         10.5265
---- EQU EQU41           .            .            .          0.0175
---- EQU EQU42           .            .            .         35.7200
---- EQU EQU43           .            .            .         45.2379
---- EQU EQU44           .            .            .        304.2000
---- EQU EQU45           .            .            .            EPS
---- EQU EQU46           .            .            .            EPS
---- EQU EQU47           .            .            .            EPS
---- EQU EQU48           .            .            .         10.5257
---- EQU EQU49           .            .            .         10.5257
---- EQU EQU50           .            .            .         10.5265
---- EQU EQU51           .            .            .          0.0175
---- EQU EQU52           .            .            .         35.7200
---- EQU EQU53           .            .            .         45.2379
---- EQU EQU54           .            .            .        304.2000
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                    LOWER        LEVEL        UPPER       MARGINAL

---- EQU EQU55           .            .            .            EPS
```

---- EQU EQU56	.	.	.	EPS
---- EQU EQU57	.	.	.	10.5257
---- EQU EQU58	.	.	.	10.5257
---- EQU EQU59	.	.	.	10.5265
---- EQU EQU60	.	.	.	0.0175
---- EQU EQU61	.	.	.	35.7200
---- EQU EQU62	.	.	.	45.2379
---- EQU EQU63	.	.	.	304.2000
---- EQU EQU64	.	.	.	EPS
---- EQU EQU65	.	.	.	EPS
---- EQU EQU66	.	.	.	EPS
---- EQU EQU67	.	.	.	10.5160
---- EQU EQU68	.	.	.	0.0175
---- EQU EQU69	.	.	.	10.5257
---- EQU EQU70	.	.	.	10.5257
---- EQU EQU71	.	.	.	EPS
---- EQU EQU72	.	.	.	EPS
---- EQU EQU73	.	.	.	EPS
---- EQU EQU74	.	.	.	EPS
---- EQU EQU75	.	.	.	EPS
---- EQU EQU76	.	.	.	EPS
---- EQU EQU77	.	.	.	EPS
---- EQU EQU78	.	.	.	EPS
---- EQU EQU79	.	.	.	EPS
---- EQU EQU80	.	.	.	EPS
---- EQU EQU81	.	.	.	0.1331
---- EQU EQU82	.	.	.	EPS
---- EQU EQU83	.	.	.	EPS
---- EQU EQU84	.	.	.	10.6428
---- EQU EQU85	.	.	.	10.6428
---- EQU EQU86	.	.	.	10.6436
---- EQU EQU87	.	.	.	0.1346
---- EQU EQU88	.	.	.	EPS
---- EQU EQU89	.	.	.	EPS
---- EQU EQU90	.	.	.	0.1171
---- EQU EQU91	.	.	.	10.5257
---- EQU EQU92	.	.	.	10.5257
---- EQU EQU93	.	.	.	10.5265
---- EQU EQU94	.	.	.	0.0175
---- EQU EQU95	.	.	.	EPS
---- EQU EQU96	.	.	.	EPS
---- EQU EQU97	.	.	.	EPS
---- EQU EQU98	.	.	.	EPS

	LOWER	LEVEL	UPPER	MARGINAL
---- EQU EQU99	.	.	.	EPS
---- EQU EQU100	.	.	.	EPS
---- EQU EQU101	.	.	.	EPS
---- EQU EQU102	.	.	.	EPS
---- EQU EQU103	.	.	.	EPS
---- EQU EQU104	.	.	.	EPS
---- EQU EQU105	.	.	.	0.0047
---- EQU EQU106	.	.	.	37.3272
---- EQU EQU107	.	.	.	45.2379
---- EQU EQU108	.	.	.	304.2000
---- EQU EQU109	.	.	.	EPS
---- EQU EQU110	.	.	.	EPS
---- EQU EQU111	.	.	.	EPS
---- EQU EQU112	.	.	.	0.0001
---- EQU EQU113	.	.	.	11.3848
---- EQU EQU114	.	.	.	38.9046
---- EQU EQU115	.	.	.	EPS
---- EQU EQU116	.	.	.	EPS
---- EQU EQU117	.	.	.	EPS
---- EQU EQU118	.	.	.	0.0001
---- EQU EQU119	.	.	.	11.3848
---- EQU EQU120	.	.	.	38.9046
---- EQU EQU121	.	.	.	EPS
---- EQU EQU122	.	.	.	EPS
---- EQU EQU123	.	.	.	EPS
---- EQU EQU124	.	.	.	EPS
---- EQU EQU125	.	.	.	EPS
---- EQU EQU126	.	.	.	EPS
---- EQU EQU127	.	.	.	EPS
---- EQU EQU128	.	.	.	0.0047
---- EQU EQU129	.	.	.	37.3272
---- EQU EQU130	.	.	.	45.2379
---- EQU EQU131	.	.	.	EPS
---- EQU EQU132	.	.	.	EPS
---- EQU EQU133	.	.	.	EPS
---- EQU EQU134	.	.	.	EPS
---- EQU EQU135	.	.	.	0.0047
---- EQU EQU136	.	.	.	37.3272
---- EQU EQU137	.	.	.	45.2379
---- EQU EQU138	.	.	.	EPS
---- EQU EQU139	.	.	.	EPS
---- EQU EQU140	.	.	.	EPS
---- EQU EQU141	.	.	.	EPS

---- EQU EQU142 . . . EPS

	LOWER	LEVEL	UPPER	MARGINAL
---- EQU EQU143	.	.	.	EPS
---- EQU EQU144	.	.	.	EPS
---- EQU EQU145	.	.	.	EPS
---- EQU EQU146	.	.	.	EPS
---- EQU EQU147	.	.	.	45.5700
---- EQU EQU148	.	.	.	38.9831
---- EQU EQU149	.	.	.	45.6193
---- EQU EQU150	.	.	.	304.2000
---- EQU EQU151	.	.	.	EPS
---- EQU EQU152	.	.	.	EPS
---- EQU EQU153	.	.	.	45.5700
---- EQU EQU154	.	.	.	45.5700
---- EQU EQU155	.	.	.	45.5700
---- EQU EQU156	.	.	.	EPS
---- EQU EQU157	.	.	.	EPS
---- EQU EQU158	.	.	.	45.5700
---- EQU EQU159	.	.	.	45.5700
---- EQU EQU160	.	.	.	45.5700
---- EQU EQU161	.	.	.	EPS
---- EQU EQU162	.	.	.	EPS
---- EQU EQU163	.	.	.	45.5700
---- EQU EQU164	.	.	.	45.5700
---- EQU EQU165	.	.	.	45.5700
---- EQU EQU166	.	.	.	EPS
---- EQU EQU167	.	.	.	EPS
---- EQU EQU168	.	.	.	EPS
---- EQU EQU169	.	.	.	EPS
---- EQU EQU170	.	.	.	EPS
---- EQU EQU171	.	.	.	45.5700
---- EQU EQU172	.	.	.	35.7200
---- EQU EQU173	.	.	.	45.2379
---- EQU EQU174	.	.	.	304.2000
---- EQU EQU175	.	.	.	EPS
---- EQU EQU176	.	.	.	EPS
---- EQU EQU177	.	.	.	35.7200
---- EQU EQU178	.	.	.	45.2379
---- EQU EQU179	.	.	.	304.2000
---- EQU EQU180	.	.	.	EPS
---- EQU EQU181	.	.	.	EPS
---- EQU EQU182	.	.	.	304.2000
---- EQU EQU183	.	.	.	304.2000
---- EQU EQU184	.	.	.	304.2000
---- EQU EQU185	.	.	.	EPS
---- EQU EQU186	.	.	.	EPS

	LOWER	LEVEL	UPPER	MARGINAL
---- EQU EQU187	.	.	.	304.2000
---- EQU EQU188	.	.	.	304.2000
---- EQU EQU189	.	.	.	304.2000
---- EQU EQU190	.	.	.	EPS
---- EQU EQU191	.	.	.	EPS
---- EQU EQU192	.	.	.	EPS
---- EQU EQU193	.	.	.	EPS
---- EQU EQU194	.	.	.	EPS
---- EQU EQU195	.	.	.	304.2000
---- EQU EQU196	.	.	.	1.0000
---- EQU EQU197	.	.	.	EPS
---- EQU EQU198	.	.	.	EPS
---- EQU EQU199	.	.	.	EPS
---- EQU EQU200	.	.	.	EPS
---- EQU INEQU1	15.0000	19.8879	+INF	.
---- EQU INEQU2	75.0000	75.0000	+INF	EPS
---- EQU INEQU3	60.0000	60.0000	+INF	EPS
---- EQU INEQU4	30.0000	30.0000	+INF	EPS
---- EQU INEQU5	.	0.1284	+INF	.
---- EQU INEQU6	10.0000	10.0000	+INF	EPS
---- EQU INEQU7	.	0.6914	+INF	.
---- EQU INEQU8	.	0.2348	+INF	.
---- EQU INEQU9	50.0000	50.0000	+INF	EPS
---- EQU INEQU10	.	.	+INF	.
---- EQU OBJNAME	.	.	.	1.0000

	LOWER	LEVEL	UPPER	MARGINAL
---- VAR F03	200.0000	205.0000	205.0000	9.0390
---- VAR F04	160.0000	165.3950	170.0000	.
---- VAR F07	4240.0000	4240.3949	4300.0000	.
---- VAR F08	4240.0000	4240.3949	4300.0000	.
---- VAR F09	4240.0000	4240.3949	4300.0000	.
---- VAR F10	4240.0000	4242.9999	4300.0000	.
---- VAR F11	4240.0000	4242.9999	4300.0000	.

---- VAR F12	4240.0000	4242.9999	4300.0000	.
---- VAR F13	3890.0000	3892.8210	3950.0000	.
---- VAR F14	3850.0000	3850.0000	3900.0000	-0.1171
---- VAR F16	3850.0000	3850.0000	3900.0000	.
---- VAR F17	40.0000	42.8210	45.0000	.
---- VAR F18	330.0000	347.2487	360.0000	.
---- VAR F19	170.0000	178.1740	190.0000	.
---- VAR F20	170.0000	178.1740	190.0000	.
---- VAR F21	12.0000	13.0600	14.0000	.

	LOWER	LEVEL	UPPER	MARGINAL
---- VAR F23	12.0000	13.0600	14.0000	.
---- VAR F24	160.0000	165.1140	190.0000	.
---- VAR F25	170.0000	181.9526	190.0000	.
---- VAR F26	160.0000	161.0942	165.0000	.
---- VAR F27	160.0000	161.0942	165.0000	.
---- VAR F28	160.0000	161.0942	165.0000	.
---- VAR F29	10.0000	20.0000	20.0000	.
---- VAR F31	10.0000	20.0000	20.0000	.
---- VAR F32	0.8000	0.9009	1.0000	.
---- VAR F33	0.8000	0.9009	1.0000	.
---- VAR FCW1	22000.0000	23751.7907	24000.0000	.
---- VAR FCW2	22000.0000	23751.7907	24000.0000	.
---- VAR FCW3	9600.0000	9600.0000	9800.0000	EPS
---- VAR FCW4	9600.0000	9600.0000	9800.0000	.
---- VAR FCW5	3350.0000	3416.2254	3450.0000	.
---- VAR FCW6	3350.0000	3416.2254	3450.0000	.
---- VAR FCW7	75.0000	80.0000	85.0000	EPS
---- VAR FCW8	75.0000	80.0000	85.0000	.
---- VAR T03	540.0000	550.0000	560.0000	EPS
---- VAR T04	560.0000	570.0000	580.0000	EPS
---- VAR T07	605.0000	624.6017	625.0000	.
---- VAR T08	1120.0000	1125.0000	1130.0000	EPS
---- VAR T09	1175.0000	1185.0000	1195.0000	.
---- VAR T10	1195.0000	1200.0000	1205.0000	.
---- VAR T11	670.0000	690.0000	690.0000	EPS
---- VAR T12	590.0000	600.0000	610.0000	.
---- VAR T13	590.0000	600.0000	610.0000	EPS
---- VAR T14	590.0000	600.0000	610.0000	.
---- VAR T16	620.0000	630.0000	640.0000	EPS
---- VAR T17	590.0000	600.0000	610.0000	.
---- VAR T18	815.0000	825.0000	835.0000	EPS
---- VAR T19	665.0000	675.0000	685.0000	EPS
---- VAR T20	560.0000	570.0000	580.0000	.
---- VAR T21	560.0000	570.0000	580.0000	.
---- VAR T23	560.0000	570.0000	580.0000	EPS
---- VAR T24	560.0000	570.0000	580.0000	.
---- VAR T25	840.0000	850.0000	860.0000	EPS
---- VAR T26	715.0000	725.0000	735.0000	EPS
---- VAR T27	715.0000	725.0000	735.0000	EPS
---- VAR T28	545.0000	550.0000	555.0000	EPS
---- VAR T29	820.0000	830.0000	840.0000	EPS
---- VAR T31	825.0000	835.0000	845.0000	EPS
---- VAR T32	1000.0000	1010.0000	1020.0000	EPS
---- VAR T33	580.0000	590.0000	600.0000	.

	LOWER	LEVEL	UPPER	MARGINAL
---- VAR TCW1	535.0000	540.0000	545.0000	EPS
---- VAR TCW2	555.0000	560.0000	565.0000	EPS
---- VAR TCW3	535.0000	540.0000	545.0000	EPS
---- VAR TCW4	555.0000	559.8727	565.0000	.
---- VAR TCW5	535.0000	540.0000	545.0000	.
---- VAR TCW6	555.0000	560.0000	565.0000	EPS
---- VAR TCW7	535.0000	540.0000	545.0000	EPS
---- VAR TCW8	555.0000	560.4050	565.0000	.
---- VAR OBJVAR	-INF	1402.2768	+INF	.
---- VAR EFF_AN	0.0001	16.5640	+INF	.
---- VAR EFF_DPA	0.0001	0.0521	+INF	.
---- VAR EFF_H2	0.0001	1.9190	+INF	.
---- VAR EFF_H2O	0.0001	0.7617	+INF	.
---- VAR EFF_N2	0.0001	0.0249	+INF	.
---- VAR EFF_NH3	0.0001	95.3167	+INF	.
---- VAR EFF_PH	0.0001	0.8663	+INF	.
---- VAR F03NH3	0.0001	205.0000	+INF	.
---- VAR F04PH	0.0001	165.3950	+INF	.
---- VAR F07AN	0.0001	13.3023	+INF	.
---- VAR F07DPA	0.0001	0.0394	+INF	.
---- VAR F07H2	0.0001	461.4728	+INF	.
---- VAR F07H2O	0.0001	17.9297	+INF	.
---- VAR F07N2	0.0001	153.8243	+INF	.
---- VAR F07NH3	0.0001	3421.7733	+INF	.
---- VAR F07PH	0.0001	172.0533	+INF	.
---- VAR F08AN	0.0001	13.3023	+INF	.
---- VAR F08DPA	0.0001	0.0394	+INF	.

---- VAR F08H2	0.0001	461.4728	+INF	.
---- VAR F08H2O	0.0001	17.9297	+INF	.
---- VAR F08N2	0.0001	153.8243	+INF	.
---- VAR F08NH3	0.0001	3421.7733	+INF	.
---- VAR F08PH	0.0001	172.0533	+INF	.
---- VAR F09AN	0.0001	13.3023	+INF	.
---- VAR F09DPA	0.0001	0.0394	+INF	.
---- VAR F09H2	0.0001	461.4728	+INF	.
---- VAR F09H2O	0.0001	17.9297	+INF	.
---- VAR F09N2	0.0001	153.8243	+INF	.
---- VAR F09NH3	0.0001	3421.7733	+INF	.
---- VAR F09PH	0.0001	172.0533	+INF	.
---- VAR F10AN	0.0001	174.2130	+INF	.
---- VAR F10DPA	0.0001	0.8562	+INF	.
---- VAR F10H2	0.0001	466.6054	+INF	.
---- VAR F10H2O	0.0001	181.2908	+INF	.
---- VAR F10N2	0.0001	155.5351	+INF	.

	LOWER	LEVEL	UPPER	MARGINAL
---- VAR F10NH3	0.0001	3255.8072	+INF	.
---- VAR F10PH	0.0001	8.6921	+INF	.
---- VAR F11AN	0.0001	174.2130	+INF	.
---- VAR F11DPA	0.0001	0.8562	+INF	.
---- VAR F11H2	0.0001	466.6054	+INF	.
---- VAR F11H2O	0.0001	181.2908	+INF	.
---- VAR F11N2	0.0001	155.5351	+INF	.
---- VAR F11NH3	0.0001	3255.8072	+INF	.
---- VAR F11PH	0.0001	8.6921	+INF	.
---- VAR F12AN	0.0001	174.2130	+INF	.
---- VAR F12DPA	0.0001	0.8562	+INF	.
---- VAR F12H2	0.0001	466.6054	+INF	.
---- VAR F12H2O	0.0001	181.2908	+INF	.
---- VAR F12N2	0.0001	155.5351	+INF	.
---- VAR F12NH3	0.0001	3255.8072	+INF	.
---- VAR F12PH	0.0001	8.6921	+INF	.
---- VAR F13H2	0.0001	466.6054	+INF	.
---- VAR F13H2O	0.0001	18.1291	+INF	.
---- VAR F13N2	0.0001	155.5351	+INF	.
---- VAR F13NH3	0.0001	3252.5514	+INF	.
---- VAR F14H2	0.0001	461.4728	+INF	.
---- VAR F14H2O	0.0001	17.9297	+INF	.
---- VAR F14N2	0.0001	153.8243	+INF	.
---- VAR F14NH3	0.0001	3216.7733	+INF	.
---- VAR F16H2	0.0001	461.4728	+INF	.
---- VAR F16H2O	0.0001	17.9297	+INF	.
---- VAR F16N2	0.0001	153.8243	+INF	.
---- VAR F16NH3	0.0001	3216.7733	+INF	.
---- VAR F17H2	0.0001	5.1327	+INF	.
---- VAR F17H2O	0.0001	0.1994	+INF	.
---- VAR F17N2	0.0001	1.7109	+INF	.
---- VAR F17NH3	0.0001	35.7781	+INF	.
---- VAR F18AN	0.0001	174.2130	+INF	.
---- VAR F18DPA	0.0001	0.8562	+INF	.
---- VAR F18H2O	0.0001	163.1617	+INF	.
---- VAR F18NH3	0.0001	0.3256	+INF	.
---- VAR F18PH	0.0001	8.6921	+INF	.
---- VAR F19AN	0.0001	9.1020	+INF	.
---- VAR F19H2O	0.0001	168.1906	+INF	.
---- VAR F19NH3	0.0001	0.3501	+INF	.
---- VAR F19PH	0.0001	0.5312	+INF	.
---- VAR F20AN	0.0001	9.1020	+INF	.
---- VAR F20H2O	0.0001	168.1906	+INF	.
---- VAR F20NH3	0.0001	0.3501	+INF	.

	LOWER	LEVEL	UPPER	MARGINAL
---- VAR F20PH	0.0001	0.5312	+INF	.
---- VAR F21AN	0.0001	7.8278	+INF	.
---- VAR F21H2O	0.0001	5.0457	+INF	.
---- VAR F21NH3	0.0001	0.0245	+INF	.
---- VAR F21PH	0.0001	0.1620	+INF	.
---- VAR F23AN	0.0001	7.8278	+INF	.
---- VAR F23H2O	0.0001	5.0457	+INF	.
---- VAR F23NH3	0.0001	0.0245	+INF	.
---- VAR F23PH	0.0001	0.1620	+INF	.
---- VAR F24AN	0.0001	1.2743	+INF	.
---- VAR F24H2O	0.0001	163.1449	+INF	.
---- VAR F24NH3	0.0001	0.3256	+INF	.
---- VAR F24PH	0.0001	0.3692	+INF	.
---- VAR F25AN	0.0001	172.7567	+INF	.
---- VAR F25DPA	0.0001	0.8562	+INF	.
---- VAR F25H2O	0.0001	0.0168	+INF	.
---- VAR F25PH	0.0001	8.3229	+INF	.
---- VAR F26AN	0.0001	159.4544	+INF	.
---- VAR F26H2O	0.0001	0.0168	+INF	.

---- VAR F26PH 0.0001 1.6230 +INF .
---- VAR F27AN 0.0001 159.4544 +INF .
---- VAR F27H2O 0.0001 0.0168 +INF .
---- VAR F27PH 0.0001 1.6230 +INF .
---- VAR F28AN 0.0001 159.4544 +INF .
---- VAR F28H2O 0.0001 0.0168 +INF .
---- VAR F28PH 0.0001 1.6230 +INF .
---- VAR F29AN 0.0001 13.3023 +INF .
---- VAR F29DPA 0.0001 0.0394 +INF .
---- VAR F29PH 0.0001 6.6583 +INF .
---- VAR F31AN 0.0001 13.3023 +INF .
---- VAR F31DPA 0.0001 0.0394 +INF .
---- VAR F31PH 0.0001 6.6583 +INF .
---- VAR F32AN 0.0001 0.0425 +INF .
---- VAR F32DPA 0.0001 0.8168 +INF .
---- VAR F32PH 0.0001 0.0416 +INF .
---- VAR F33AN 0.0001 0.0425 +INF .
---- VAR F33DPA 0.0001 0.8168 +INF .
---- VAR F33PH 0.0001 0.0416 +INF .
---- VAR FEED_AN 0.0001 1.2655 +INF .
---- VAR FEED_DPA 0.0001 0.0024 +INF .
---- VAR FEED_H2 0.0001 1.8990 +INF .
---- VAR FEED_H2O 0.0001 0.0754 +INF .
---- VAR FEED_N2 0.0001 0.0246 +INF .
---- VAR FEED_NH3 0.0001 100.2370 +INF .

LOWER LEVEL UPPER MARGINAL

---- VAR FEED_PH 0.0001 17.1589 +INF .
---- VAR H03 -9999.0000 -3.9924 +INF .
---- VAR H04 -9999.0000 -6.5790 +INF .
---- VAR H07 -9999.0000 -72.1825 +INF .
---- VAR H08 -9999.0000 -49.9070 +INF .
---- VAR H09 -9999.0000 -44.9980 +INF .
---- VAR H10 -9999.0000 -44.9980 +INF .
---- VAR H11 -9999.0000 -70.0944 +INF .
---- VAR H12 -9999.0000 -78.6489 +INF .
---- VAR H13 -9999.0000 -63.9998 +INF .
---- VAR H14 -9999.0000 -63.2958 +INF .
---- VAR H16 -9999.0000 -62.3089 +INF .
---- VAR H17 -9999.0000 -0.7040 +INF .
---- VAR H18 -9999.0000 -7.0107 +INF .
---- VAR H19 -9999.0000 -16.9449 +INF .
---- VAR H20 -9999.0000 -20.3804 +INF .
---- VAR H21 -9999.0000 -0.2229 +INF .
---- VAR H23 -9999.0000 -0.2229 +INF .
---- VAR H24 -9999.0000 -16.8330 +INF .
---- VAR H25 -9999.0000 9.2943 +INF .
---- VAR H26 -9999.0000 7.4851 +INF .
---- VAR H27 -9999.0000 7.4851 +INF .
---- VAR H28 -9999.0000 6.2547 +INF .
---- VAR H29 -9999.0000 0.5404 +INF .
---- VAR H31 -9999.0000 0.5463 +INF .
---- VAR H32 -9999.0000 0.1053 +INF .
---- VAR H33 -9999.0000 0.0759 +INF .
---- VAR PROFIT 0.0001 1402.2768 +INF .
---- VAR Q100 -9999.0000 25.0965 +INF .
---- VAR Q101 -9999.0000 4.9090 +INF .
---- VAR Q102 -9999.0000 8.5545 +INF .
---- VAR Q103 -9999.0000 3.4356 +INF .
---- VAR Q104 -9999.0000 1.2304 +INF .
---- VAR Q105 -9999.0000 0.0294 +INF .
---- VAR TE100 . 70.0896 +INF .
---- VAR TE102 . 90.5340 +INF .
---- VAR TE103 . 63.2991 +INF .
---- VAR TE104 . 55.2908 +INF .
---- VAR TE105 . 181.9381 +INF .

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OBJVAR objective or profit function
EFF_AN
EFF_DPA
EFF_H2
EFF_H2O
EFF_N2
EFF_NH3
EFF_PH
F03NH3
F04PH
F07AN
F07DPA
F07H2
F07H2O
F07N2
F07NH3
F07PH
F08AN
F08DPA
F08H2
F08H2O
F08N2
F08NH3
F08PH
F09AN
F09DPA
F09H2
F09H2O

F09N2
F09NH3
F09PH
F10AN
F10DPA

F10H2
F10H2O
F10N2
F10NH3
F10PH
F11AN
F11DPA
F11H2
F11H2O
F11N2
F11NH3
F11PH
F12AN
F12DPA
F12H2
F12H2O
F12N2
F12NH3
F12PH
F13H2
F13H2O
F13N2
F13NH3
F14H2
F14H2O
F14N2
F14NH3
F16H2
F16H2O
F16N2
F16NH3
F17H2
F17H2O
F17N2
F17NH3
F18AN
F18DPA
F18H2O
F18NH3
F18PH
F19AN

F19H2O
F19NH3
F19PH
F20AN
F20H2O
F20NH3
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F21AN
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F21PH
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F23H2O
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F25DPA
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F25PH
F26AN
F26H2O
F26PH
F27AN
F27H2O
F27PH
F28AN
F28H2O
F28PH
F29AN
F29DPA
F29PH
F31AN
F31DPA
F31PH
F32AN
F32DPA
F32PH
F33AN
F33DPA
F33PH
FEED_AN
FEED_DPA

FEED_H2
FEED_H2O
FEED_N2
FEED_NH3
FEED_PH
H03
H04
H07
H08
H09
H10
H11
H12
H13
H14
H16
H17
H18
H19
H20
H21
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H24
H25
H26
H27
H28
H29
H31
H32
H33
PROFIT
Q100
Q101
Q102
Q103
Q104
Q105
TE100
TE102
TE103
TE104
TE105

**** REPORT SUMMARY : 0 NONOPT
0 INFEASIBLE
0 UNBOUNDED
0 ERRORS

EXECUTION TIME = 0.060 SECONDS 0.7 Mb WIN-18-097

USER: Ralph W. Pike G990726:1450AP-WIN
Louisiana State University, Department of Chemical EngineeriDC267

**** FILE SUMMARY

INPUT C:\PROGRAM FILES\ADVANCED PROCESS ANALYSIS SYSTEM\GAMS25\DO_ECON
OUTPUT C:\PROGRAM FILES\ADVANCED PROCESS ANALYSIS SYSTEM\GAMS25\DO_ECON.LST
SAVE C:\PROGRAM FILES\ADVANCED PROCESS ANALYSIS SYSTEM\GAMS25\PUT_DATA.G0?